Strong Correlations in Ultracold Fermi Gases

Dissertation

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Abstract

Ultracold atomic gases provide an ideal system with which to study fundamental many-body physics. Exhibiting universal interactions in clean and controllable environments, long-used simple models as well as more exotic models can now be realized. The interplay between theory and experiment is therefore very active, and, in this thesis, I will detail several works, both exact analytic results and numerical calculations, which have impacts on current experiments. I begin with an introduction to the field including a brief discussion of experiments, the microscopic model of two species of interacting fermions, the BCS-BEC crossover and an overview of the various phases of atomic Fermi gases. I then describe the various results of my theoretical investigations, which are divided into five chapters. First, I describe radio frequency (RF) spectroscopy experiments and how they probe the single-particle spectral function. This leads to my results on an exact feature of the spectral lineshape, a universal large-momentum structure which exists for all states of interacting Fermi systems and has been verified in recent angle-resolved RF experiments. Second, I focus on gases which have a normal Fermi liquid ground state and show that their lineshape exhibits a characteristic jump discontinuity. I illustrate this Fermi surface singularity and the previously mentioned universal large momentum tail with explicit calculations. Third, I turn to the low energy structure of the single-particle spectral function in the superfluid state. I argue that sharp low energy quasiparticle excitations exist across the BCS-BEC crossover using a general argument that includes the interaction of fermions with the low-energy collective mode. This is illustrated with an explicit calculation within an approximation scheme. Fourth, I address the trap-induced inhomogeneity and use a Bogoliubov-deGennes analysis to test if a simple local density approximation (LDA) can provide an adequate description of a spin imbalanced Fermi system. Finally, I discuss dynamics of atomic gases motivated by a recent experiment in which two spin-polarized clouds are allowed to collide with each other. Despite the underlying attractive interactions, the clouds are seen to bounce off of each other. Using a hydrodynamic description, I argue that the short and intermediate time dynamics reflects a metastable state in which the effective interaction is repulsive. It is my hope that the work presented in this thesis can be used to gain key insights which inspire future endeavors.
To Chase, whose presence in my life has enriched me more than I could have imagined.
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Chapter 1
INTRODUCTION

Ultracold atomic gases are very remarkable physical systems. With both bosonic and fermionic species available for cooling well below degeneracy, simple interactomic interactions, and precise control of their environment available, one can realize many fundamental hamiltonians which occur in condensed matter. This allows one to study a wide variety of many body physics. In this introductory chapter, we will begin this thesis with an introduction to the field and the parameters of the experimental system. We will then give the current understanding of the phases of matter that fermions exhibit which we will study. Finally, we give an outline of the results in this thesis.

The 1980’s and early 1990’s saw a tremendous advancement in the cooling of alkali atoms, earning S. Chu, C. Cohen-Tannoudji and W. Phillips the 1997 Nobel prize in physics. This allowed physicists to study quantum behavior of a macroscopic number of atoms. In 1995 these techniques proved sufficient enough to achieve Bose-Einstein condensation (BEC) in $^{85}$Rb, earning W. Ketterle, C. Weiman and E. Cornell the 2001 Nobel Prize in physics and verifying the prediction made by Bose and Einstein 70 years prior. The gases obtained were shown to have particle densities of the order of $10^{13} - 10^{15} \text{ cm}^{-3}$ at temperatures less than the degeneracy temperature of $\sim 10^{-5} \text{ K}$. For comparison, air at standard temperature and pressure is about $10^{22} \text{ cm}^{-3}$ and for nuclear matter $10^{38} \text{ cm}^{-3}$. The Fermi temperature for electrons is of order $10^4 - 10^5 \text{ K}$ while for helium degeneracy is achieved below 1 K. Many phenomena were studied in boson systems, including condensate interference, vortex creation and collective mode behavior. Soon fermions enjoyed degenerate temperatures for the first time at JILA [7], starting an intense study of cold fermions.

There are several advantages to studying quantum phenomena in cold atomic gases. Firstly, the gases are dilute in the sense that the interatomic interaction has a range $r_0$ of the order of 50 Å while the interatomic spacing is of the order of 1000 Å, and therefore many quantities are insensitive to those microscopic details. There is therefore a kind of “universality” in the system, meaning $^6\text{Li}$ has the same behavior as $^{40}\text{K}$, save for mass differences. However, interactions play a fundamental role despite this diluteness, as exhibited
by the many phenomena that occur. Practically, these are attractive systems since their manipulation and observation [1] can be done using lasers and magnetic fields, providing a clean and controllable environment. Numbers of particles, spin imbalance, and interparticle interactions are easily tuned, all in contrast with condensed matter.

Theoretically, the advantages come from the simple definition of the physical system, namely, the small range of the interactions $V_{\text{int}}(r)$ providing a description in terms of the low energy scattering length $a_s$ between atoms and a known background potential $V_{\text{trap}}(r)$. For single-spin bosons, which exhibit BEC, in which all bosons occupy the same single particle state, may be described in terms of the Gross-Pitaevskii equations, a weakly interacting theory [8]. Fermions under ambient magnetic field also behave weakly – even noninteracting if there is only one spin component. However, with two spins of fermions the scattering length can actually be tuned using a simple magnetic field to yield arbitrarily strong interactions, called a “Feshbach” resonance. This provides a way of probing strong correlations in Fermi gases, where analytical theories cease to provide a complete description, but nevertheless can still give deep insights.

In this introductory chapter we will first discuss some of the atomic physics and the formalism we will use to describe it, and then turn to the main physical regime of this thesis, the BEC-Bardeen-Cooper-Schrieffer (BCS) crossover. We end with an outline of the results in the thesis.

1.1 Ultracold Atoms

The remarkable control of atomic gases in the experiments comes from the use of lasers and magnetic fields, and in this section we briefly describe the manipulation relevant for the experiments which we will reference in this thesis. The first traps included both optical and magnetic trapping, although here we will be concerned only with optical traps since we want to save the magnetic field for the tuning of Feshbach resonances. Laser light with an energy of order the optical range interacts with cold atoms via the AC Stark shift, the laser creating a spatially varying but time-averaged electric field $E(r)$ due to the fact that the time scale for the motion of the atoms is much slower than the inverse frequency $\omega_L^{-1}$ of the light. The coupling is therefore $-\vec{d} \cdot E(r)$. At frequencies in the vicinity of the transition $\omega_0$ from the atom’s ground state $^2S_{1/2}$ to the excited state $^2P_{1/2}$, but far from the linewidth $\Gamma$ of the transition ($\Gamma \ll |\omega_L-\omega_0| \ll \omega_0$), the energy shift can be calculated using second order perturbation theory and has the form

$$V_{\text{trap}}(r) = \frac{1}{2} \alpha(\omega_L)||E(r)||^2,$$  \hspace{1cm} (1.1)
Figure 1.1: Hyperfine energies for $^6$Li (right) and $^{40}$K (left) measured from the ground state energy without the hyperfine coupling. The splittings at zero field $\nu_{rf}$ are 228 MHz and -1.286 GHz for $^6$Li and $^{40}$K, respectively (Note: $h\nu_{hf} = (i + 1/2)A$ where $i = 1, 4$ for $^6$Li and $^{40}$K, respectively). Figure obtained from ref. [1].

where $\alpha(\omega_L)$ is the polarizability of the atom, given by

$$\alpha(\omega_L) \simeq \frac{|\langle e|\hat{d}|g\rangle|^2}{\hbar(\omega_0 - \omega_L)},$$

(1.2)

ignoring transitions to other states. Using a focussed laser beam along the z-direction, the intensity $|E(r)|^2$ has a maximum, and the trap potential becomes approximately harmonic:

$$V_{\text{trap}}(r) \simeq -V_0 + \frac{1}{2}m\omega_r^2r^2 + \frac{1}{2}m\omega_z^2z^2,$$

(1.3)

where $\omega_r$ and $\omega_z$ are the trap frequencies and the trap depth $V_0$ ranges from 1-1000 kHz. The width of the trap has the scale of millimeters. We note that one can control the asymmetry of trap as well as its depth independently. Furthermore, one can use two counter-propagating laser beams to produce a standing wave potential, providing a lattice for the atoms of several geometries [8].

The application of a homogeneous magnetic field $\mathbf{B} = B\hat{z}$ produces the hyperfine hamiltonian for an atom with $l = 0$, $j = s = 1/2$ and nuclear spin $i = 1$

$$\hat{H}_m = A\hat{s} \cdot \mathbf{i} + \gamma_e\hbar\hat{s}_zB + \gamma_n\hbar\hat{i}_zB,$$

(1.4)

where $A$ is the hyperfine coupling and $\gamma_{e,n}$ are the gyromagnetic ratios of the electron and nuclear spins, respectively. The hamiltonian can be diagonalized with the states $|f,m_f\rangle$
with energies $E_{f,m_f}$. We refer to Fig. 1.1 for $^6\text{Li}$ and $^{40}\text{K}$. Note that in the high field “Paschen-Back” regime the lowest hyperfine states are used in experiments. We will denote the populated states by $\sigma$ and any unpopulated states being excited by $e$.

Let us now briefly discuss the interparticle interactions involved in ultracold atoms, since they are crucial for tuning [2, 9]. We restrict ourselves to a three-dimensional, two-component, single-species Fermi gas with dominant $s$-wave interactions. The interparticle potential $V_{\alpha,\beta}(r)$ depends on the relative distance $r$ between the atoms, the relative angular momentum, and is a matrix in the pair of hyperfine spins of the two atoms collectively called a “channel” and denoted by $\alpha \equiv \{f_1, m_{f_1}, f_2, m_{f_2}, l, m_l\}$. For large distances, the potential behaves as $-C_6/r^6$ independent of the hyperfine state, where the $C_6$ coefficient serves as an experimentally-determined parameter. The corresponding “true” range of the potential can be defined by $r_0 \equiv (mC_6/\hbar^2)^{1/4}$, and is again on the order of 10 Å as mentioned above. At shorter distances, however, the electron clouds of the atoms start to overlap, causing a strong repulsion. The spin states of the two atoms and the coupling of every channel must be taken into account in principle to solve the scattering problem. We will, however, see that we don’t need to know every matrix element for an adequate description. In fact, due to the low temperature of the gas, we can solve the Schrödinger equation for the two atoms at low momentum, and, using standard scattering theory, one obtains the scattering amplitude

$$f(k) = \frac{1}{-1/a_s + r^*k^2 + ik},$$

(1.5)

where $r^*$ is the effective range of the potential, and $a_s$ the scattering length. In most cases $r^*$ is of the same order as the true range $r_0$, and can be neglected if the diluteness condition, $k_F r_0 \ll 1$, is satisfied. In this case, we see the merit that any short-range model can be used for the same Fermi gas, as long as it produces the same scattering length. We will therefore not write down explicit formulas for the full potential curves.

To illustrate how this coupling between different channels produces a resonance, we first note that the Schrödinger matrix contains a relatively decoupled subset of the original populated channel and another unpopulated one for certain choices of magnetic field ranges. We therefore restrict ourselves to these two channels. Plotted qualitatively in Fig. 1.2, the “open” or “background” channel potential $V_{bg}(r)$ is the appropriate diagonal part of $V_{\alpha,\beta}(r)$ which would occur in the absence of the resonance. The “closed” channel $V_c(r)$ is so called since it approaches a finite constant for large $r$. We will furthermore assume that only a single bound state $\lambda_{cl}(r)$ in one other channel is the dominant term, owing to the small difference in energy between the initial scattering energy and the bound state energy. The appropriate off-diagonal coupling term will be denoted $W(r)$. We subsequently rewrite the
The Schrödinger equation as a two-channel model:

\[
\begin{pmatrix}
H_{bg}(r) & W(r) \\
W(r) & H_{cl}(B, r)
\end{pmatrix}
\begin{pmatrix}
\lambda_\alpha(r) \\
\lambda_{cl}(r)
\end{pmatrix} = E
\begin{pmatrix}
\lambda_\alpha(r) \\
\lambda_{cl}(r)
\end{pmatrix},
\]  

(1.6)

where \(H_{bg}(r)\) is the single channel hamiltonian for the entrance channel in the absence of any coupling, and \(H_{cl}(B, r)\) is the closed channel hamiltonian with the magnetic field shift included. The off-diagonal coupling \(W(r)\), is real and short-ranged. Solving for the corresponding scattering amplitude we obtain the generic form Eq. (1.5), where the effective range \(r^*\) depends on the strength of \(W\). The scattering length obtains the form

\[
a_s = a_{bg} \left(1 - \frac{\Delta B}{B - B_0}\right),
\]  

(1.7)

where \(\Delta B\), which depends on \(r^*\) and the magnetic moment \(\mu\) of the closed channel, is the width of the resonance and \(a_{bg}\) the background scattering potential which occurs in the absence of the Feshbach resonance. We then find that the diverging of the scattering length is a product of the crossing of a bound level in a different channel with the scattering energy of the original populated channel. This is similar to shape resonances, in which bound or quasi-bound states occur in the original scattering potential.
1.2 The Many-Body Problem

In this section we show how we model the short-distance behavior in the many body problem. By using the Bethe-Peierls condition

$$\lim_{r \to 0} \left[ \frac{1}{r} \frac{d}{dr} (r \phi(r)) \right] = \frac{1}{a_s},$$

which amounts to enforcing the limit

$$\phi(r) \sim \frac{1}{r} - \frac{1}{a_s} \quad \text{as } r \to 0,$$

where the proportionality constant depends on the normalization, we only need the scattering length to describe the interactions described in the previous section. The corresponding condition on the many-body wavefunction $\Psi(\{r_i\})$ is

$$\Psi(r_1, \ldots, r_i, \ldots, r_j, \ldots, r_N) = \sum_{P_k} (-1)^{P_k} \left[ \frac{1}{|r_i - r_j|} - \frac{1}{a_s} \right] \chi_{i,j} \Psi'(\{r_i\}),$$

where $|r_i - r_j| \to 0$, $\chi$ is the spin wavefunction, and $\Psi'$ does not depend on $r_i$, $r_j$. It is understood that the other $N - 2$ particles are kept fixed. We can build this into our hamiltonian by considering a pseudopotential of the form $-g \Lambda \delta(r_i - r_j)$, where $\Lambda \sim 1/r^*$ is a momentum cutoff which must be “regularized” in momentum-space expressions, since any physical potential decreases for sufficiently large momentum. Analogously to Eq. (1.9), we use the vacuum Lippman-Schwinger equation

$$T_{k',k}(E) = V_{k',k} + \sum_{k''} V_{k',k''} G^0(k'', E) T_{k'',k}(E),$$

where $G^0(k, E) = 1/(E + i0^+ - 2\epsilon_k)$ is the Green’s function for the free propagation of the pair, to determine the $T$ matrix which is related to the scattering amplitude by

$$f(k) = -\frac{m}{4\pi \hbar^2} T_{k,k} \left( E = \frac{\hbar^2 k^2}{m} \right).$$

Using our pseudopotential and taking the limit $k \to 0$, we obtain

$$\frac{m}{4\pi a_s} = -\frac{1}{g \Lambda} + \sum_{|k|<\Lambda} \frac{1}{2\epsilon_k},$$

where we’ve explicitly restricted the momentum integral because it diverges as $\Lambda$. We therefore keep $g \Lambda$ finite and restrict all momentum integrals until the final expressions.
where we then allow $\Lambda \to \infty$. Our many-body hamiltonian, then, becomes

$$\hat{H} = \sum_{\sigma} \int d^3x \psi_\sigma^\dagger (x) \left( -\frac{\nabla^2}{2m} - \mu_\sigma \right) \psi_\sigma (x) - g_\Lambda \int d^3x \psi_\uparrow^\dagger (x) \psi_\downarrow^\dagger (x) \psi_\downarrow (x) \psi_\downarrow (x).$$

(1.14)

In momentum space, it becomes

$$\hat{H} = \sum_{k,\sigma} \xi_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} - \frac{g_\Lambda}{V} \sum_{k,k',Q} c_{k+Q,\uparrow}^\dagger c_{-k',\downarrow}^\dagger c_{-k',\downarrow} c_{k+Q,\uparrow},$$

(1.15)

where $\xi_{k,\sigma} \equiv \epsilon_k - \mu_\sigma$ and $V$ is the total volume. We note that, following normal conventions for lack of better notation, $V$ is used here for volume. We will in this thesis usually set the volume to be unity, using context to determine when it appears.

The restriction of momentum sums to momenta with magnitude less than $\Lambda$ is only necessary for certain quantities which are then “sensitive” to the details of the interatomic potential. For example, the hamiltonian above does not need the restriction due to a cancellation of the kinetic and potential energies which are separately sensitive. Consequently, the free energy per particle $F(T,V,N)/N = \epsilon_F \bar{F}(T/T_F, 1/k_F a_s)$, where $\bar{F}$ is a dimensionless function which is independent of the microscopic details to order $(k_F r^*)^2$. Any Fermi atom should then be described by the same function when properly scaled. For any dynamic quantities, such as the spectral function or the radio frequency (RF) spectrum to be introduced later, we are restricted to momenta and energies less than the corresponding quantity related to $\Lambda$.

### 1.3 BEC-BCS crossover

The BEC-BCS crossover is the physical regime of interactions of two-spin fermions in which the scattering length of the fermions, $a_s$, is tuned to arbitrary values. We compare the scattering length with the Fermi wavevector $k_F$ of the fermions, defined by $k_F^3/3\pi^2 = n$, where $n$ is the particle density. This then defines the interaction parameter $k_F a_s$ which can take all values, $(-\infty, \infty)$. Since the unitary regime occurs when the scattering length diverges, we also use $1/k_F a_s$ as an interaction parameter. Weak coupling then corresponds to $1/k_F a_s \gg 1$ and negative, while strong coupling corresponds to $1/k_F a_s \gg 1$ and positive. The term “strong interactions” corresponds to the unitary regime where $1/k_F a_s \ll 1$.

#### 1.3.1 BCS-Leggett Mean Field Theory

To begin understanding the physics of fermions in the BEC-BCS crossover, we will review BCS-Leggett theory [12], which gives a good qualitative understanding of the ground state. The basic idea comes from the Cooper problem: that a pair of fermions in states $(k, \uparrow)$ and $(-k, \downarrow)$, where $|k| \simeq k_F$, can bind in 3D under infinitesimally weak attractive interactions
with an energy lower than the noninteracting Fermi gas. In metals, this attraction is given by a phonon-mediated process between electrons. In atoms, this attraction is given naturally as explained in the previous section. It is natural, then, to write down the $N$-particle wavefunction

$$
\Psi_{MF}(\{r_i\}, N) = \sum_{P_k} (-1)^{P_k} \prod_{i<j} \phi(r_i - r_j) \chi_{i,j}
$$

as a product of $N/2$ pair wavefunctions $\phi(r)\chi_{i,j}$ (appropriately antisymmetrized under all permutations $P_k$), where $\phi$ and $\chi = (|↑↓⟩ - |↓↑⟩)/\sqrt{2}$ are the (symmetric) orbital and (antisymmetric) spin parts, respectively. The noninteracting limit corresponds to the limit as $\phi$ turns into a pair of plane wave states. To show the lowering of the ground state energy with respect to pairing we calculate the ground state energy by considering the BCS interaction hamiltonian, which is a restriction of Eq. (1.15) to exclude all $|Q| > 0$, anticipating that zero-momentum pairs constitute the main portion of the pairing. We have

$$
\hat{V}_{MF} = -\frac{g_{\Lambda}}{V} \sum_{k,k'} c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger c_{-k',\downarrow}^\dagger c_{k',\uparrow}.
$$

This can be solved as a variational minimization by considering the grandcanonical version of Eq. (1.16), in second quantized form,

$$
|\Psi_{MF}\rangle = \prod_k \left( u_k + v_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger \right) |\text{vac}\rangle.
$$
Minimizing \( \langle \Psi_{MF} | \hat{H}_{MF} | \Psi_{MF} \rangle \) with respect to \( u_k, v_k \) such that \( u_k^2 + v_k^2 = 1 \) (the normalization condition), we find that the thermodynamic potential

\[
\Omega_0(\mu, T = 0) = -|\Delta_0|^2 \frac{m}{4\pi\hbar^2 a_s} - \sum_k \left( E_k - \xi_k - \frac{|\Delta_0|^2}{2\epsilon_k} \right),
\]

(1.19)

where \( \Delta_0 \) satisfies the “gap equation”

\[
\frac{m}{4\pi a_s} = \sum_k \left( \frac{1}{2\epsilon_k} - \frac{1}{2E_k} \right),
\]

(1.20)

and \( E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta_0^2} \). One can show that the thermodynamic potential here is less than that for a noninteracting Fermi gas throughout the entire coupling range, and is therefore a better ground state. The quantity \( \Delta_0 \), which depends on \( u_k, v_k \), serves as an order parameter for the gas, being zero in the normal state and becoming nonzero as one decreases the temperature. In terms of the Fermi operators, \( \Delta_0 = -g_A \sum_k \langle c_{k,1} c_{-k,1} \rangle = g_A \sum_k u_kv_k \), and therefore is an amplitude for removing a pair of particles from the system with opposite momenta. Together with the number equation, \( n = -\partial \Omega_0 / \partial \mu = 2 \sum_k v_k^2 \), the solutions for \( \Delta_0 \) and \( \mu \) are plotted in Fig. 1.3.

In order to get a feeling for the nature of the gas, let us focus on limiting cases. The weak coupling regime defined by \( k_F a_s < 0 \) and \( k_F |a_s| \ll 1 \) is called the BCS regime, since it gives similar results as for the original problem in typical superconductors. The order parameter \( \Delta_0 = 8\epsilon_F \exp(\pi/2k_F a_s) / e^2 \) is an exponentially different scale than the Fermi energy, and therefore not a perturbative result. The ground state energy becomes \( E_{BCS} = E_{FG} - 3N \Delta_0^2 / 8\epsilon_F \). We see that, from Fig. 1.4, that the energy \( E_k \) is different from the noninteracting excitation energy only in a small region of momentum, and, similarly, that the momentum distribution is different from the noninteracting one in the same region. To illustrate the spatial structure of the pairs, we can calculate their size \( r_{\text{pair}} = \sqrt{\langle r^2 \rangle} \). We find that \( r_{\text{pair}} = k_F / m \Delta_0 \), which is exponentially large. This gives the picture that the gas is composed of Fermi pairs near the Fermi energy with an exponentially small binding energy. We note that what we have not included are fluctuations in the pairing states, which give rise to Fermi liquid corrections \([13]\). We also note that scattering due to polarization of the medium \([14]\) reduces the gap by a numerical factor.

In the strong coupling limit, the fermions bind together, such that, in Eq. (1.16), each \( \phi \) is a bound state of two fermions, and has the form \( \phi \sim e^{-r/a_s} / r \). From our crossover theory, the chemical potential is simply \( \mu = -E_0 / 2 + \pi \hbar^2 a_s n / m \), which is half the binding energy of a dimer with the mean field contribution between dimers and can be obtained through a bosonic theory of \( N/2 \) dimers. The pair size is shown in Fig. 1.5 by the dashed lines. There is a smooth evolution from the BCS limit, where the size is much bigger than the interparticle spacing, \( k_F r_{\text{pair}} \gg 1 \), to the strong coupling limit where \( r_{\text{pair}} = a_s \ll k_F^{-1} \),
characteristic of strong bound pairs. We note that what this crossover theory does not included are fluctuations in the pairing, which gives rise to collective modes in the system. In the BEC limit, these modes correspond to a further interaction between pairs and give rise to a Bogoliubov Bose gas with scattering length \( a_{dd} \approx 0.55a_s \) [13] between dimers. By solving exactly the four-particle Schrödinger equation, \( a_{dd} = 0.6a_s \) [15].

The intermediate region when \( k_F a_s \gg 1 \) defines the “unitary” region, and is characterized by the absence of a small parameter. The only length scale in the problem is then \( k_F \), and therefore the free energy per particle is a universal function \( \epsilon_F \tilde{F}(T/T_F, 0) \) of \( T/T_F \). This region then has a second kind of universality in which even the scattering length does not determine its properties. We finally note that there is no phase transition for any value of the coupling \( k_F a_s \) – it is simply a crossover. In the crossover theory above, the quasiparticle weights, \( u_k^2 \) and \( v_k^2 \), are indeed finite throughout the crossover and all experiments to date have not seen evidence of singularities characteristic of quantum phase transitions. We will address this question later in Chapter 4.

### 1.3.2 Finite Temperature

We can further illustrate the BEC-BCS crossover by increasing the temperature, shown in the phase diagram in Fig. 1.5. Generalizing the previous discussion, we obtain corrections the thermodynamic potential (1.19), gap equation (1.20), and number equation. In the weak coupling BCS limit the situation is clear: a second order transition at \( T_c = \epsilon_F \exp(\pi/k_F a_s) \) separates the superfluid state from a normal Fermi liquid, and the form of \( T_c \) indicates that the transition is due simply to pair breaking via thermal fluctuations. On the strong coupling side the mean field physics we have included is only due to pairing, and therefore
Figure 1.5: Qualitative phase diagram for spin-balanced Fermi gases in the BEC-BCS crossover with interaction parameter $1/k_Fa_s$. At zero temperature the average pair size is illustrated by red and blue dots joined by dashed lines. The yellow superfluid region is bounded above by the normal Fermi liquid, pseudogap, and normal Bose liquid in the BCS, unitary, and BEC regions, respectively. The dashed line increasing from left to right indicates the pairing temperature $T^*$. Figure obtained from Ref. [3].
the transition is predicted to occur at $T^* \sim E_b \ln(\frac{E_b}{\epsilon F})^{3/2}/2$ involving the binding energy. We, however, can intuitively find an inconsistency with this, by considering that if we have composite bosons we should expect a transition temperature proportional to the density, so that $T_c = \bar{\hbar}^2 [n_B/\zeta(3/2)]^{2/3}/m_B$. This is because we expect that the bosons are condensed, and the transition occurs not because of pair breaking, but of thermal fluctuations kicking whole pairs to higher momentum states. The gas can then be considered a thermal Bose gas. If we include in our theory these collective modes of the bosons [16, 17], we would indeed obtain this result but $m_B = 2m$ and $n_B = n/2$.

At unitarity, again, the critical temperature is of the order of the Fermi temperature, $T_c \sim T_F$, and Quantum Monte Carlo (QMC) calculations [18–20] point to a prefactor of 0.15 - 0.20. We point out that this ratio $T_c/T_F$ is the highest of any other phase of matter, and is a novel aspect of ultracold fermions. The nature of the gas above $T_c$ is, however, only recently understood. Since the natures of the gas above $T_c$ in both the weak and strong coupling sides are very different, we can guess that this region at unitarity is quite complicated. The transition is certainly still associated with the loss of off-diagonal long-range order (ODLRO), but, as we’ve seen in the two limits, the existence of a pairing gap does not have to coincide with the transition. In fact, one finds that there is still strong pairing at unitarity causing a gap in the spectrum. The existence of this gap was found [21] to exist in the single particle spectrum.

### 1.3.3 Polarized Fermi gases

A novel aspect of ultracold atomic systems is the tuning of spin imbalance in the system. Since the ground state for a spin-balanced system is a superfluid of pairs, polarization inherently breaks up the Cooper pairs in the system and competes with superfluidity. The spin imbalance [22, 23] is described by an effective magnetic field $h \equiv (\mu_\uparrow - \mu_\downarrow)/2$, resulting in two different Fermi surfaces. Once Cooper pairs are broken, superfluidity is lost and a normal Fermi liquid develops, upon a critical field $h_c = \Delta/\sqrt{2}$ at a first order transition. Experimental hints at coexistence of superfluidity and the normal phase [24–26] were observed through discontinuities in the spatial profile of trapped gases, with a superfluid core and normal edges. By inducing vortices in the superfluid core, it was shown [24] that, indeed, there is a transition. A phase diagram [4, 27] at unitarity also found the critical polarization $P = 0.40$ at zero temperature, as shown in Fig. 1.6. From QMC calculations [5], it has been determined at unitarity that the ground state is indeed a Fermi liquid for a polarization $P > 0.40$ by comparing the Fermi liquid energy with that of the balanced superfluid.

One useful way of thinking about the phase diagram is to consider the limit of full polarization. The BEC limit is perhaps the most accessible, since the pairing is so strong that extra fermions simply immerse themselves in the bosonic sea, interacting with an atom-
Figure 1.6: Experimental measurement [4] of the phase diagram for polarized Fermi gases for temperature $T$ and polarization $P = (n_\uparrow - n_\downarrow) / (n_\uparrow + n_\downarrow)$ at unitarity ($1/k_F a_s = 0$). The filled symbols indicate experimental measurements of the density distributions of the atoms. Open symbols indicate theoretical calculations. Particularly, the open square at $P \approx 0.40$ is the calculation of Lobo et al. [5].
dimer scattering length $a_{ad} \simeq 1.1a_s$ [28]. In the limit of full polarization, we have a single bound boson in a sea of Fermi atoms. Indeed, by considering the fully polarized case, it was shown [29, 30] that a single down spin in a sea of up spins can be described by a variational wavefunction of the form

$$|\Psi_{\text{polaron}}\rangle = \varphi_0 c_{0,\downarrow}^\dagger |\Psi_0\rangle + \sum_{p,q} \varphi_{p,q} c_{q-p,\downarrow}^\dagger c_{p,\uparrow}^\dagger |\Psi_0\rangle,$$

where $\varphi_0$ and $\varphi_{p,q}$ are the amplitudes of the minority spin to be in the respective momentum states and, since $|\Psi_0\rangle$ is a noninteracting state, the momentum sum is restricted to $|p| > k_F$, $|q| < k_F$. The state has an energy above the noninteracting energy $E_{FG}$ of $|\Psi_0\rangle$ that evolves from the mean field energy $-\frac{4\hbar^2}{m} n_\uparrow a_s$ in the BCS limit to a large binding energy $-E_b$ in the BEC limit. At unitarity the value is still strong, $-0.6\epsilon_F$. More exact calculations [31, 32] confirm this result and find a transition between the Fermi polaron and molecule at a value of $1/k_Fa_s \simeq 0.90$.

1.4 Metastable Ferromagnetic State

Up to this point we have described the paired superfluid and normal Fermi liquid ground states of interacting Fermi gases. An interesting question is whether - in the presence of strong repulsive interactions - one can find a ferromagnetic state of fermions. From theoretical work dating back to the 1930s (see Ref. [33] and Sec. 11.7 in Ref. [34]) it was argued that itinerant fermions with short range repulsion might undergo a ferromagnetic Stoner instability. This instability should cause the fermions to separate into spin-polarized domains in which the potential energy is zero, energetically more favorable than the initial interaction energy.

A recent experiment from the Ketterle group at MIT [35] claimed to have seen such an instability in ultracold gases. However, the effective repulsion in this system comes from being on the upper branch of the Feshbach resonance, an excited state with scattering length $a_s > 0$ for which the ground state is the BEC side of the BEC-BCS crossover. Thus, the question of how long this metastable excited state can live before decaying to the lower branch is crucial. If a quasi-equilibrium state could be maintained in the upper branch, then QMC calculations [36, 37] showed that, for many observables, the upper branch physics would look very much like a repulsive Fermi system. However, it appears that the timescales for remaining on the upper branch in the original MIT experiment are very short [38] and no clear evidence for a ferromagnetic state is observed.

In the last part of this thesis, we turn to a remarkable new dynamical experiment from the Zwierlein group at MIT, which we show is related to a metastable ferromagnetic state in a very interesting way. An important feature of ultracold atom experiments is that one can prepare dynamical experiments arbitrarily far from equilibrium. In the Zwierlein
experiment [6], two spin-polarized clouds were prepared in a spatially separated manner and then allowed to collide under the effect of the trapping potential. For weak interactions, the clouds pass through each other, as one might expect. The relative center of mass of the two clouds oscillates around the center of the trap. The most unexpected result is that, for strong interactions, the clouds repel each other at short times, bouncing off of each other. We show in Chapter 6 that the reason why the clouds bounce off of each other, despite the underlying attraction, is related to the effective repulsion on the upper branch of the Feshbach resonance. The unusual short and intermediate time bounce dynamics is argued to be related to a metastable ferromagnetic state in the system.

1.5 Outline of the Thesis

We will now give an outline of this thesis in order to summarize the findings. In chapter 2 we discuss the universal structure of the single particle spectral function for large momentum, namely, that for hole-like excitations at momentum \( k \gg k_F \) the dominant weight occurs at \( \omega \approx -\frac{\hbar^2 k^2}{2m} \), a feature which is immediately familiar only with superfluid phases of matter. We show here that this feature is, in fact, not associated with pairing or even attraction, occurring in repulsive Fermi gases as well as attractive ones. We understand this feature is a result of phase space restrictions on two-particle propagation, and verify that its integral corresponds with general considerations on the momentum distribution \( n_k \). Our prediction of this large-\( k \) universal feature has been verified by angle-resolved RF experiments [39].

In chapter 3, we derive general features for the RF spectrum. First, at low energies in normal Fermi liquids there is a jump discontinuity usually associated with the momentum distribution \( n_k \). We next derive the form for a high-energy tail connected with the large-\( k \) behavior of the spectral function \( A \) in the previous chapter and again find another relation involving Tan’s constant \( C \). We then illustrate our general results by approximate calculations which show the merits and disadvantages of two approximation schemes used in the literature to calculate the full lineshape of the RF spectrum with these general features in mind.

In chapter 4, we turn to the low energy part of the superfluid spectral function and address a fundamental question: whether there are sharp quasiparticles in the system, i.e., singular peaks in \( A(k, \omega) \). There have been conflicting works on this point. We give a general argument considering the coupling of the fermions to the low energy collective mode in the system. We show that there are indeed sharp quasiparticles across the entire BEC-BCS crossover. We use the gaussian approximation to the partition function to illustrate this general result and analyze how fluctuations in the order parameter shift the dispersion.

In chapter 5, we address the inhomogeneity of the atomic clouds by an explicit cal-
calculation of the densities \( n_\sigma(x) \) and order parameter \( \Delta(x) \) of the system. We use the Bogoliubov-deGennes (BdG) equations, an inhomogeneous mean field theory which is the simplest theory beyond the local density approximation (LDA). We analyze the regions inside the cloud in order to interpret the results of two conflicting experiments. We find that order parameter oscillations must be interpreted with care, as a finite numerical cutoff can lead to misleading conclusions. We find that the LDA may fail for sufficiently small numbers of particles and strong asymmetry.

Finally, in chapter 6, as in Sec. 1.4 above, we consider the collision of two clouds of atomic Fermi gases prepared in different spin states close to a Feshbach resonance, motivated by the recent experiment of Sommer et al. [6]. We argue that, upon coming into contact with each other, the fermions in the strongly interacting regime are well described by hydrodynamics. Solving Euler’s equations, we show that the clouds bounce off each other, with a damped oscillatory motion of the two centers of mass at short time, followed by phase separation of the two species at intermediate times. These dynamics, which are in excellent agreement with the experiment, reflect a metastable many-body state on the “upper branch” of the resonance where the effective interaction is repulsive, despite the underlying attraction.
The spectral function \( A(k, \omega) = -\text{Im} G(k, \omega + i0^+)/\pi \) of the single-particle Green’s function \( G \) is of fundamental interest in many-body physics [40]. In addition to information about the spectrum and dynamics of single-particle excitations, it is also directly related to thermodynamic functions of a many-particle system. Very recently there has been experimental progress in measuring (the occupied part of) \( A(k, \omega) \) in strongly interacting Fermi gases [8, 41], using a momentum-resolved version [42] of radio frequency (RF) spectroscopy [43–45]. These measurements [42] of \( A(k, \omega) \) for ultracold atomic gases are the analog of angle-resolved photoemission, which has given deep new insights into novel materials.

In this chapter\(^1\) we describe remarkable universal large-\( k \) structure of \( A(k, \omega) \) for dilute gases with observable effects in RF experiments. Our investigation was motivated by the elucidation of the universal ultraviolet structure of equal-time correlations by Tan [10, 11, 47–50]. One of his central results is the universal \( k \gg k_F \) behavior of the momentum distribution \( n_\sigma(k) \simeq C/k^4 \), where \( C \) is the “contact” [10, 11, 47–50]. Using the \( T = 0 \) sum rule \( \int_{-\infty}^{0} d\omega A(k, \omega) = n(k) \), this necessarily implies that \( A(k, \omega) \) has weight below the chemical potential (\( \omega < 0 \)) for \( k \gg k_F \). This is “incoherent” spectral weight, not associated with the coherent Landau quasiparticle. We will show that

- The incoherent part of the \( \omega \) vs. \( k \) dispersion when \( k \gg k_F \) goes like \( -\epsilon(k) = -k^2/2m \), “bending back” away from the chemical potential at large \( k \).
- While this back-bending is expected in BCS theory and its generalizations for a paired superfluid, we argue that this unusual dispersion is a universal feature of all dilute Fermi gases, even those with a normal (non-superfluid) ground state.
- We find that the spectral weight of \( C/k^4 \) in \( A(k, \omega) \) is centered about \( \omega \simeq -\epsilon(k) \) in a range of energies of order \( v_F k \) for normal Fermi gases. Most of the spectral weight \( (1 - C/k^4) \) is, of course, centered about \( \omega \approx +\epsilon(k) \), but these states are not occupied.

\(^1\) This work was done in collaboration with M. Randeria and published in Physical Review A [46].
and do not contribute to $n(k)$.

This bending back is clearly visible in the data of Ref. [42] for attractive fermions near unitarity and near or above $T_c$. However, it is hard to separate the effects of the finite temperature pairing pseudogap [51] and normal state interaction effects. In particular, a bending back of the dispersion above $T_c$ cannot by itself be used as evidence for a pairing pseudogap in view of the normal state results described below.

We will first introduce radio frequency spectroscopy in general and then focus on two systems where the ground state is a normal Fermi liquid: (a) the hard-sphere dilute Fermi gas, and (b) the highly imbalanced attractive Fermi gas. We then turn to the superfluid ground state, where we will argue that, in the BCS limit, the unusual dispersion is dominated by interaction effects rather than the effect of pairing. We conclude with implications for RF spectroscopy experiments.

## 2.1 Radio Frequency Spectroscopy

One major tool of manipulating the atoms between different hyperfine states is RF spectroscopy, in which in addition to the optical trap the atoms are subject to a RF pulse in the $x$ direction which transfers one of the hyperfine spins $\sigma$ in the system to a third unoccupied state $e$. The RF field couples to the electrons in the form $\hat{H}_{\text{rf}} = -\gamma_e \hbar \sum_i \hat{S}_{i,x} B_{\text{rf}} e^{i\omega_L t}$, where we neglect the nuclear coupling since $\gamma_n \ll \gamma_e$. Furthermore, since we are interested only in the transition between $\sigma$ and $e$, we will ignore all other transitions. Further details are in [52]. We can therefore incorporate the probe as a perturbation of the form

$$\hat{H}_{\text{rf}}(t) = \gamma \int d^3x \left( e^{-i\omega_L t} \psi_e^\dagger(x) \psi_\sigma(x) + e^{i\omega_L t} \psi_\sigma^\dagger(x) \psi_e(x) \right),$$

valid for laser frequencies $\omega_L$ near the transition of interest, $\omega_{\sigma,e}$. The coupling constant $\gamma$ contains the dipole matrix element and the power of the laser, and $\omega_L$ is the laser frequency. To measure the response, we measure the rate of production of $e$ atoms, $\dot{N}_e \equiv dN_e/dt = i[\hat{H}_{\text{rf}}(t), \hat{N}_e]$. In the event that $\gamma$ is small, we can use linear response theory to determine the spectrum. The RF response is then proportional to the imaginary part of the corresponding correlation function

$$\Pi^R(x - x', t - t') = -i\theta(t - t') \langle \left[ \psi_\sigma^\dagger(x, t) \psi_e(x, t), \psi_e^\dagger(x', t') \psi_\sigma(x', t') \right] \rangle.$$

(2.2)

After a Fourier transform, we obtain

$$I_{\text{rf}}(\omega) = -2\gamma^2 \text{Im} \Pi^R(q = 0, \omega),$$

(2.3)

where we redefine our frequency $\omega \equiv \omega_L - \Delta E_\sigma$ where $\Delta E_\sigma$ is the difference in energy between the $e$ level and the bottom of the $\sigma$ band. The long-wavelength character is
Figure 2.1: Calculation of the correlation function $\Pi$. The upper diagram is the full calculation with all vertex corrections in the shaded box, while in the lower diagram these vertex corrections are neglected. Furthermore, the excited $e$ state can be taken to be the free-particle Green’s function, indicated by a thin line.

due to the negligible momentum transfer of the incoming photon. We note that, due to the linear response of the system, $I_{rf}$ obeys several sum rules $[10, 53, 54]$. For example, $\int_{-\infty}^{\infty} d\omega I_{rf} = 2\pi \gamma^2 n_\sigma$. We will discuss the sum rules in detail in Chapter 3.

We will, in this thesis, ignore interactions of the final state $e$ with the other spin state in the system. This is because we are interested in the macroscopic physics of the initial system, and not with the probe we use to measure them. If these interactions are strong one must take into account vertex corrections $[55]$ to accurately model the experimental lineshapes. We can then factorize Eq. (2.2) to obtain

$$I_{rf}(\omega) = 2\pi \gamma^2 \sum_k A_\sigma(k, \xi_k, \sigma - \omega) (f(\xi_k, \sigma) - f(\xi_k, e)), \quad (2.4)$$

represented diagrammatically in Fig. 2.1. The function $A_\sigma(k, \omega)$ is the single particle spectral function, defined as $-\text{Im } G(k, \omega)/\pi$, where $G$ is the Green’s function

$$G(k, t) = -\left\langle T \left( c_{k,\sigma}^\dagger(t) c_{k,\sigma}^\dagger(0) \right) \right\rangle. \quad (2.5)$$

The Green’s function contains all the single particle dynamics and provides crucial information about the nature of the excitations in a many body system $[40]$, and the spectral function $A$ can be interpreted as the probability that a certain excitation with momentum $k$ and energy $\omega$ can be made. In a normal phase, we only need to calculate Eq. (2.5). From general considerations in a Fermi liquid, the spectral function has the form

$$A^{FL}(k, \omega) = Z \delta(\omega - \xi_{k,\sigma}) + A^{inc}(k, \omega), \quad (2.6)$$

where the quasiparticle weight $Z < 1$ indicates the gapless excitations in the system. For a superfluid phase, the ODLRO means we also have the “anomalous” Green’s function

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for the operator $c_{k,\uparrow}e_{-k,\downarrow}$. We will defer the discussion of $F^0$ to Chapter 4. Now, within BCS-Leggett theory, we have

$$G^0(k, \omega) = \frac{u_k^2}{\omega + i0^+ - E_k} + \frac{v_k^2}{\omega + i0^+ + E_k},$$

(2.7)

and the spectral function

$$A^0(k, \omega) = u_k^2 \delta(\omega - E_k) + v_k^2 \delta(\omega + E_k)$$

(2.8)

is then sharply peaked resulting in very large (in fact, infinite) lifetimes for the excited states with energy $E_k$. This, then, gives the picture that the gas is composed of infinitely long lived quasiparticles. In fact, the limit as $\Delta_0 \to 0$ gives precisely the truly noninteracting Green’s function. At the bottom of the dispersion, the quasiparticle weights, $u_k^2, v_k^2$, are each 1/2. One can view the superfluid state as having split the noninteracting excitation with weight 1 into two gapped excitations for particles and holes.

We now have a simple physical interpretation of RF spectroscopy – a momentum sum over all probabilities $A$ of energetically allowed transitions weighted by the occupation of levels with energy $\xi_{k,\sigma} - \omega$. We can then use our calculations of $A$ and perform the necessary convolution to obtain $I_{rf}$. We also note that, since the $e$ state is unoccupied in the experiments, $f(\xi_{k,e}) \equiv 0$.

In order to illustrate the RF spectrum we first note that the noninteracting limit when $A(k, \omega) = \delta(\omega - \xi_{k,\sigma})$ gives a $\delta$-function: $I_{rf} = 2\pi \gamma^2 n_{\sigma} \delta(\omega)$, where $\omega = \omega_L - \epsilon_{F,\sigma}$. For weak interactions such that one can use mean field physics, we get the same expression, only the frequency is shifted from the noninteracting value by $-2\pi \hbar^2 n_{\sigma} (a_s - a_s^{'})/m$. Including the Galitskii-Lee-Yang corrections [56, 57] results in a broadened lineshape, and we will address this for normal gases in this chapter. Finally, the crossover theory in the superfluid from the Introduction results in a lineshape with a threshold occurring at $E_0 - \mu_{\sigma}$.

Experimentally, absorption images of the $\sigma$ or $e$ states reveal the total number of fermions transferred. Early experiments in $^6$Li [43, 58] attempted to measure the pairing gap, however, inhomogeneity and final state interactions obscured the results. By choosing a different set of initial hyperfine states in $^6$Li or by using $^{40}$K, it was shown that final state interactions can be minimized. Moreover, a tomographic technique allows one to get better spatial resolution [59]. It was furthermore shown in Ref. [42] that, if one resolves the momentum profile of the resulting gas one instead measures the integrand in Eq. (2.4), $A(k, E)f(E)$, which is the occupied part of the spectral function with energy $E = \xi_k - \mu_{\sigma} - \omega$. This is in analogy to angle-resolved photoemission spectroscopy where the chemical potentials play the role of the work function. The momentum $k$ can be measured precisely, but, unfortunately, the chemical potential cannot be measured, so one instead measures the spectral function with respect to the energy of the free Fermi gas, since it is
2.2 Dilute Repulsive Fermi Gas

We begin with the simplest example of a normal Fermi liquid: 3-dimensional hard sphere Fermi gas with mass \( m \) and scattering length \( a > 0 \) with \( na_s^3 \ll 1 \). Of course, here \( a_s = r_0 \), the range, and the “large” \( k \) regime where \( n(k) \sim k^{-4} \) is \( k_F \ll k < 1/r_0 \). Thus, unlike Ref. [11], where \(|a_s| \gg r_0\), we cannot set \( r_0 = 0 \). However, we can still use the short range regularization we introduced in the Introduction. The Fermi liquid thermodynamic and Fermi-liquid properties were studied by Galitskii and Lee, Yang and Huang; see Sec. 5 of [40]. The high-\( k \) tail was also calculated [60] and is

\[
n(k) \simeq (k_F a)^2 \left( \frac{2}{3\pi} \right)^2 \left( \frac{k_F}{k} \right)^4.
\]

(2.9)

To calculate the self energy, we note that in the low density limit \( na_s^3 \ll 1 \), the most important physical process is repeated scattering in the particle-particle channel. Diagrammatically, we obtain the corresponding sum of ladder diagrams \( \Gamma \) illustrated by Fig. 2.2. Analytically, we obtain for \( \Gamma \),

\[
\Gamma^{-1}(Q) = \frac{1}{g} - L(Q) \quad L(Q) = \sum_k \frac{1}{2\epsilon_k} + T \sum_{k,n} G^0(k + Q)G^0(-k)
\]

(2.10)

where \( Q = (Q, iQ_\ell) \) with \( iQ_\ell = i2\ell\pi T \) and \( k = (k, ik_n) \) with \( ik_n = i(2n + 1)\pi T \). The bare Green’s function \( G^0(k) = 1/[ik_n - \xi(k)] \) and we have replaced the bare interaction \( g\Lambda \) with the scattering length via Eq. (1.13). Note that one can obtain an analytically closed form expression [61] for \( L(Q, \Omega + i0^+) \), which we state for reference at the end of this chapter. For the hard sphere Fermi gas we can use the approximation \( \Gamma \approx g + g^2 L \), where \( g \equiv 4\pi a h^2 / m \),
Figure 2.3: Left: Logarithmic intensity plot of $A(k, \omega)\epsilon_F/(k_F a_s)^2$ for the repulsive Fermi gas ($k_F a = 0.1; na_s^3 = 3.4 \times 10^{-5}$). The most intense (red) line at $\omega \approx \xi_k$ is the quasiparticle. We focus on the unusual dispersion centered about $\omega = -\epsilon(k)$ (black dashed line) in the range $\omega = -\epsilon(k) - 3\epsilon_F \pm 2v_F k$ (white dashed lines); see text. Right: Momentum distribution tail for the same gas.

which amounts to second order perturbation theory. The Matsubara self-energy is

$$\Sigma_{\sigma}(k, ikn) = \frac{1}{\beta} \sum_{q,l} \Gamma(q, iq_l) G(q - k, iq_l - ikn)$$  \hspace{1cm} (2.11)

and, after performing the Matsubara sum and analytically continuing, $\Sigma(k, ikn \to \omega + i0^+) = \text{Re}\Sigma + i\text{Im}\Sigma$, where

$$\text{Im}\Sigma(k, \omega) = \sum_q \text{Im}\Gamma(k + q, \omega + \xi(q)) [\Theta(-\xi(q)) - \Theta(-\omega - \xi(q))]$$  \hspace{1cm} (2.12)

at $T = 0$. Re$\Sigma$ is obtained numerically by a Kramers-Kronig transform on Im$\Sigma$ by

$$\text{Re}\Sigma(k, \omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} dz \frac{\text{Im}\Sigma(k, z)}{\omega - z}$$  \hspace{1cm} (2.13)

due to the analytic properties of the self energy. We note that, in the case of the simplification $\Gamma \approx g + g^2L$ for the hard sphere gas, this expression for the self energy is valid only for $\omega \ll 1/m a_s^2$. Im$\Sigma$ grows indefinitely for larger $\omega$. We subtract out this singular behavior $S(z) = -i(2\sqrt{2}/3\pi)(k_F a)^2\sqrt{\epsilon_F z}$ and then Kramers-Kronig transform Im$\Sigma = \text{Im}\Sigma - \text{Im}S$.

The real self-energy is then Re$\Sigma = \text{Re}\Sigma + \text{Re}S$.

The spectral function is plotted in Fig. 2.3 on a logarithmic scale. We see the most intense feature, corresponding to the Landau quasiparticle near $k_F$, tracks $\omega \approx +\xi(k)$, up to many-body renormalizations. We have checked our numerics against known results [40] for chemical potential $\mu$, quasiparticle residue $Z$, effective mass $m^*$, and the scattering rate near the Fermi surface. However our main interest is in the much less intense, incoherent
spectral feature that follows an $\omega = -\epsilon(k)$ dispersion and dominates $n(k)$ at large $k$.

To understand this “bending back”, we need to determine when $\text{Im}\Sigma(k,\omega)$ is non-zero for $k \gg k_F$ and $\omega < 0$. To understand our result qualitatively, consider the diagram in Fig. 2.4. The dominant contribution comes from small values of both $|Q|$ and $\Omega$ of the effective interaction $\Gamma$. (For large values of these variables there is no spectral weight $\text{Im}\Gamma$ for two-particle scattering.) Thus $q \simeq -k$ and $\omega \simeq -\xi(q) \simeq -\epsilon(k)$ for $k \gg k_F$. This shows that $A \neq 0$ for $\omega$ around negative $\epsilon(k)$.

To make this more quantitative, we use Eq. (2.12). From the structure of $L(Q,\Omega)$, it follows that $\text{Im}\Gamma(Q,\Omega) \neq 0$ when $\Omega \geq \Omega_0(Q) \equiv \min_p \{\xi(p+Q/2)+\xi(-p+Q/2)\} = \epsilon(Q)/2 - 2\mu$; see Fig. 2.4. From the difference of $\Theta$-functions, $k_F \leq q \leq q_{\text{max}}(\omega) \equiv k_F [1 + |\omega|/|\epsilon_F|]^{1/2}$. This implies that $-|\omega| \leq \Omega \leq 0$. Together with the kinematical constraint $|k - q| \leq Q \leq k + q$, this leads to $Q_{\text{min}} = |k - q_{\text{max}}(\omega)|$. For non-zero $\text{Im}\Sigma$ we thus need the kinematically allowed region (shaded rectangle in Fig. 2.4) to overlap with $\Omega \geq \Omega_0(Q)$. This leads to the simple condition $Q_{\text{min}} \leq Q_0$, where the definition $\Omega(Q_0) = 0$ leads to $Q_0 = 2k_F$. (We have also found, but do not discuss here, the $\omega > 0$ threshold for $A \neq 0$.)

Solving $|k - q_{\text{max}}(\omega)| = 2k_F$, we find $A(k,\omega < 0) \neq 0$ in the range of energies $\omega = -\epsilon(k) - 3\epsilon_F \pm 2v_F k$; see Fig. 2.3. For $k \gg k_F$, this simplifies to $|\omega + \epsilon(k)| \leq 2v_F k$. Although the width of this range grows linearly with $k$, it becomes small relative to the central energy which grows like $-k^2$ for large $k$. We plot in Fig. 2.3 the $n(k)$-tail using $\int_{-\infty}^0 d\omega A(k,\omega)$ and find that it agrees with the analytical result [60]. The incoherent spectral weight in $A(k \gg k_F,\omega)$ in the interval $|\omega + \epsilon(k)| \leq 2v_F k$ is thus precisely $(2k_F a/3\pi)^2(k_F/k)^4$. 

Figure 2.4: Top: Kinematics of the processes that contribute to imaginary self-energy in Eq. (2.12). $\text{Im}\Sigma$ is non-zero when the shaded rectangle (allowed by kinematics and thermal factors) overlaps with the region $\Omega > \Omega_0(Q)$ (in which $\text{Im}\Gamma$ is non-zero). This leads to the condition $Q_{\text{min}} \leq Q_0$. Bottom: Diagram contributing to $\text{Im}\Sigma$. 

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2.3 Highly Imbalanced Normal Fermi Gas

We next turn to a two-component attractive Fermi gas with scattering length $a$ tuned through a broad Feshbach resonance. Here we can indeed consider $|a_s| > r_0$ and we set the range $r_0 = 0$. While the ground state for equal spin populations is a superfluid exhibiting the BCS-BEC crossover, we consider the different regime of large spin imbalance $n_\uparrow/n_\downarrow$.

There is by now considerable theoretical [5, 29, 62–64] and experimental evidence [44, 45] that, for sufficiently large imbalance, superfluidity is destroyed for a large range of values of $a_s$, including unitarity $|a_s| = \infty$, and the ground state is a (partially polarized) normal Landau Fermi liquid.

For large $|a_s|$, we use the number of fermion species $2\mathcal{N}$ with a $Sp(2\mathcal{N})$-invariant interaction as an artificial parameter to control the calculation in a large-$\mathcal{N}$ expansion [61–63]. Beginning with the Hamiltonian of the $\mathcal{N}$ fermions,

$$\hat{H}_{\mathcal{N}} = \sum_{i=1}^{\mathcal{N}} \int d^3x \psi_{i,\sigma}^\dagger(x) \left(-\frac{\nabla^2}{2m} - \mu_{i,\sigma}\right) \psi_{i,\sigma}(x) - \frac{g_\Lambda}{\mathcal{N}} \sum_{i,j=1}^{\mathcal{N}} \int d^3x \psi_{i,\uparrow}^\dagger(x) \psi_{i,\downarrow}^\dagger(x) \psi_{j,\downarrow}(x) \psi_{j,\uparrow}(x), \quad (2.14)$$

we write down the Green’s function of the $\sigma$ fermions of interest

$$G_{\sigma}(k, \tau) = -\left\langle T \left( \psi_{\sigma}(k, \tau) \psi_{\sigma}^\dagger(k, 0) \right) \right\rangle, \quad (2.15)$$

and note that the relevant diagrams are again those in Fig. 2.2, since the vertices bring factors of $1/\mathcal{N}$ and the particle-particle propagation brings a factor of $\mathcal{N}$, yielding an overall factor of $1/\mathcal{N}$. To first order in $1/\mathcal{N}$, then, the resulting expression is

$$\text{Im}\Sigma(k, \omega) = \sum_\mathbf{q} \text{Im}\Gamma(k + \mathbf{q}, \omega + \xi_\uparrow(\mathbf{q})) \left[ \Theta(-\xi_\uparrow(\mathbf{q})) - \Theta(-\omega - \xi_\uparrow(\mathbf{q})) \right], \quad (2.16)$$

after setting $\mathcal{N} = 1$. This is equal to Eq. (2.12) with $\xi$ replaced by $\xi_\uparrow$ both in the $\Theta$-function and in the definition of $\Omega$.

We can again analytically determine the energy range for which $\text{Im}\Sigma$, and hence $A$, are non-zero. In Fig. 2.4 we must now use $\Omega_0(Q) \equiv \epsilon(Q)/2 - 2\mu$ with $2\mu = \mu_\uparrow + \mu_\downarrow$. The final result is that, for $k \gg k_F$ and $\omega < 0$, $A(k, \omega)$ can be non-zero only in the range of energies $|\omega + \epsilon(k)| \leq \alpha \nu_{F\uparrow}k$ where $\alpha = \sqrt{2(1 + \epsilon_{F\uparrow}/\epsilon_{F\uparrow})}$. One can obtain more stringent bounds for the imbalanced case using the detailed structure of $\text{Im}\Gamma$, but the simpler analysis described here suffices to establish a range linear in $k$ centered about $-\epsilon(k)$.

For concreteness, we focus here on unitarity $|a| = \infty$. $A(k, \omega)$ for the highly imbalanced ($n_\downarrow/n_\uparrow = 0.01$) unitary gas is shown in Fig. 2.5. We have also verified that we get a $1/k^4$
Figure 2.5: Logarithm intensity plot of \( A_k(\omega) \) for minority particles in the unitary Fermi gas with imbalance \( n_\downarrow/n_\uparrow = 0.01 \). The white dashed lines \( \omega = -\epsilon(k) \pm \alpha v_F k \) are derived in the text; the black dashed line is \( \omega = -\epsilon(k) \).

tail for \( n(k) \) in this system. Our calculation of \( A(k,\omega) \) is controlled only within the \( 1/N \)-expansion. Note, however, that the singularity structure in the large \( k \) limit is determined only by short distance properties of the two-body problem in vacuum, while the strength of the singularity \( C \) depends on the many-body state. Since the ladder approximation is exact for the two-body problem, we expect the bending back in the spectral function to be robust beyond the \( 1/N \)-expansion.

### 2.4 Superfluid State

We now turn to a discussion of the superfluid ground state for a system with equal densities of up and down spins and an interaction described by a scattering length \( a \). Unlike the normal Fermi liquids described above, a branch of the dispersion that tracks \( -\epsilon(k) \) at large \( k \) is very natural for the fermionic excitations in a superfluid [65]. Nevertheless, even in this case, our analysis gives important quantitative insights.

In BCS mean field theory the spectral function \( A_{\text{MF}}(k,\omega) = v_k^2 \delta(\omega + E(k)) + u_k^2 \delta(\omega - E(k)) \) where \( v_k^2 = 1 - u_k^2 = \frac{[1 - \xi(k)/E(k)]}{2} \). The excitation energy \( E(k) = \sqrt{\xi^2(k) + \Delta^2} \) with \( \Delta \) the energy gap. For \( k \gg k_F \), \( E(k) \approx \epsilon(k) \) and \( v_k^2 \approx \Delta^2/2\epsilon^2(k) \), so that \( A_{\text{MF}}(k \gg k_F, \omega < 0) \approx \frac{\Delta^2}{2\epsilon^2(k)} \delta(\omega + \epsilon(k)) \). Thus we see that particle-hole mixing in the superfluid ground state naturally leads to a bending back of the dispersion.

However, there is a (large) quantitative problem with this result even in the BCS limit \((1/k_F a \ll -1)\), where one might have expected it to be the most accurate. Using \( n(k) = \int_{-\infty}^{0} d\omega A(k,\omega) \), or directly from BCS theory, one finds that the momentum distribution \( n_{\text{MF}}(k) = v_k^2 \approx \frac{\Delta^2}{2\epsilon^2(k)} = C_{\text{MF}}/k^4 \) for \( k \gg k_F \). The problem is that the contact
estimated from BCS theory $C_{MF} \sim \Delta^2 \sim \exp(-1/k_F|a|)$ is exponentially small in $|a|$. However, the exact answer [10, 11, 47–50] in the BCS limit is $C = 4\pi^2n^2a^2$ as $a \to 0^-$. To understand why BCS theory gets the wrong answer for $C$ we use the adiabatic relation [11] $dE/da = \hbar^2C/(4\pi ma^2)$. As shown in [13], interaction effects lead to power-law corrections in $|a|$ in the ground state energy density $\mathcal{E}$, which are numerically much more important than the essentially singular corrections coming from pairing. In the extreme BCS limit, the contact is dominated by the Hartree term in $\mathcal{E}$ with calculable corrections [13].

Thus the actual $A(k \gg k_F, \omega < 0)$, even in the BCS limit, is dominated by interaction effects beyond BCS mean field theory. This results in a spectral weight $C \sim |a|^2$ arising from interaction effects which exist even in the normal state, rather than resulting from pairing, which only makes an exponentially small contribution. We make a final note on a work by Combescot et al. [66], where the approximation $\text{Im}\Sigma(k \gg k_F, \omega < 0) \propto \delta(\omega + \epsilon(k))$ is used which leads to a sharp feature in $A(k, \omega)$. While this may be sufficient for computing “integrated” quantities like $n(k)$, it does not capture the incoherent structure in $A(k, \omega)$ described here.

2.5 Technical Details of Effective Interaction

Here we derive the explicit expression for the effective interaction Eq. (2.10), also reported in Ref. [61]. We denote the chemical potentials inside the particle-particle vertex Im$\Gamma$ as $\mu_\sigma$. When performing the integrals in Eq. (2.10) we need to define the following functions:

$$F(\Omega) \equiv \sqrt{|\Omega - \Omega_0(Q)|}, \quad \Omega_0(Q) \equiv \epsilon_Q/2 - 2\mu$$

We write $L(Q, \Omega) \equiv L_0 + L_\uparrow + L_\downarrow$, where $L_0(Q, \Omega)$ is the nonanalytic piece given by $(m^{3/2}F(\Omega)/4\pi)[\Theta(\Omega_0(Q) - \Omega) - i\Theta(\Omega - \Omega_0(Q))]$, and give separately the formulas for the real and imaginary parts of $L_\sigma$. The imaginary part is

$$L''_\sigma(Q, \Omega) = \frac{m^{3/2}}{8\pi}F(\Omega)\Theta(\Omega - \Omega_0) \begin{cases} 
2\Theta(2k_F - Q) & \Omega \leq \Omega_0^- (Q) \\
1 - x_\sigma(Q, \Omega) & \Omega_0^- (Q) < \Omega < \Omega_0^+ (Q) \\
0 & \Omega \geq \Omega_0^+ (Q)
\end{cases}$$

where $x_\sigma(Q, \Omega) = (\Omega - 2\sigma h)\sqrt{m}/QF(\Omega)$. The real part of $L_\sigma$ is written like

$$L'_\sigma(Q, \Omega) = \frac{m^{3/2}}{8\pi^2}H_\sigma(Q, \Omega)\Theta(\mu_\sigma)$$
Figure 2.6: False color plots of \( \text{Im} \Gamma(Q, \Omega) \). Black dashed lines correspond to the lines \( \Omega_0 \) and \( \Omega_\pm^\sigma \). Blue to red indicates negative to positive values, and yellow corresponds to \( \text{Im} \Gamma = 0 \). Top: Galitskii gas for \( k_F a_s = 0.1 \). Bottom: Unitary Fermi Liquid for \( 1/a_s = 0 \) and \( n_\downarrow/n_\uparrow = 0.01 \). The dotted line indicates the pole.

where \( H_\sigma \) is

\[
H_\sigma(Q, \Omega) = \frac{2k_{F\sigma}}{\sqrt{m}} - \frac{\sqrt{m}}{Q}(\Omega - 2\sigma h) \ln \left| \frac{\Omega - \Omega_+^\sigma}{\Omega - \Omega_-^\sigma} \right| - \\
- 2F(\Omega)\Theta(\Omega_0 - \Omega) \left[ \tan^{-1} \frac{F(\Omega_+^\sigma)}{F(\Omega)} + \eta \tan^{-1} \frac{F(\Omega_-^\sigma)}{F(\Omega)} \right] + F(\Omega)\Theta(\Omega - \Omega_0) \ln \left| \frac{F(\Omega_+^\sigma) - F(\Omega)}{F(\Omega_+^\sigma) + F(\Omega)} \right| \left| \frac{F(\Omega_-^\sigma) - F(\Omega)}{F(\Omega_-^\sigma) + F(\Omega)} \right|^\eta
\]

(2.20)

where \( \eta \equiv \text{sgn} \ (2k_{F\sigma} - Q) \). In the first “self-consistent” calculation the formulas simplify because \( \mu_\downarrow < 0 \) and \( \mu_\uparrow = \epsilon_{F\uparrow} \), and therefore \( L_\downarrow \equiv 0 \). In the \( 1/N \) calculation we keep every term since the \( \mu_\sigma = \epsilon_{F\sigma} > 0 \). In the Galitskii gas, \( \mu_\uparrow = \mu_\downarrow = \epsilon_F \) and therefore \( \Omega_\uparrow^\pm = \Omega_\downarrow^\pm \).

To illustrate the vertex in both the types of normal gases we present a contour plot for the Galitskii Fermi gas and the unitary Fermi liquid for \( n_\downarrow/n_\uparrow = 0.01 \) in Fig. 2.6. We see that, indeed, for \( \Omega < 0 \) the region when \( \text{Im} \Gamma \) is finite is restricted to wavevectors and energies
of order the Fermi energy. We also see that when performing the integral in Eq. (2.12), the numerical integrations necessary to calculate $\Sigma''$ and $\Sigma'$ can be quite time-consuming unless one studies the discontinuities of the equations above, namely, $\Omega_0$ and $\Omega_{\pm}^\sigma$. Furthermore, the pole of $\Gamma$ has a dispersion which enters the incoherent weight of $\Gamma$ producing an integrable divergence.
Chapter 3

Radio Frequency Spectroscopy: Singular Features and Sum Rules

There has been intense experimental activity on characterizing various states of matter in ultracold atomic gases \([8, 41]\). This will become ever more important with the possibility of new and exotic states being realized in these systems. An important tool in these studies is radio frequency (RF) spectroscopy where an RF pulse is used to transfer atoms from one hyperfine level to another. The RF signal \([43, 67]\) has turned out to be much harder to interpret than initially thought because of complications of strong final state interactions and the inhomogeneity of trapped gases. Recently it has become possible to eliminate these problems by choice of suitable hyperfine levels (in \(^6\)Li) and by tomographic techniques that focus on specific regions of the gas. The most detailed experimental results are available for polarized Fermi gases \([44, 45]\).

Motivated by these experiments, we\(^2\) first describe two exact results for the singular features in RF spectra \(I_\sigma(\omega)\), Eq. \((2.4)\), of a two-component Fermi gas with arbitrary interactions. Our results complement the exact results on sum rules \([53, 54]\). We work in the limit where final state interaction effects are negligible, so that we can focus on the nontrivial effects of interactions in the many-body state.

- The RF spectrum \(I_{\text{rf}}(\omega)\) has a universal \(C\omega^{-3/2}\) tail at high frequencies, where \(C\) is Tan’s contact coefficient \([11, 47–49]\), which is independent of spin. This form is valid for all phases of Fermi gases: superfluid \([8, 41]\), highly imbalanced normal Fermi liquid \([5, 24, 25, 29, 45, 64, 69]\) or even a balanced Galitskii Fermi Liquid \([40]\).
- In any normal Fermi liquid state, the RF spectrum \(I(\omega)\) at \(T = 0\) has a jump discontinuity. Its location depends on the chemical potential \(\mu\) and its magnitude is determined by the combination of Fermi liquid parameters \(Z/(1 - m/m^*)\), where \(Z\) is the quasiparticle weight and \(m^*\) the effective mass.

These exact results are important not only in interpreting experiments, but also in

\(^2\)This work was done in collaboration with V. Shenoy and M. Randera and is posted on arxiv.org \([68]\).
understanding various approximation schemes [54, 55, 63], which are necessarily required to calculate the RF lineshape \( I(\omega) \) for a strongly interacting gas. In the second part of our paper we critically analyze diagrammatic approximations for the highly imbalanced normal Fermi liquid.

- We show that a simple self-consistent approximation, motivated by the fact that it is essentially exact in the \( n_\downarrow = 0 \) limit [29, 69], has serious qualitative problems for non-zero \( n_\downarrow \): The minority spins do not exhibit the universal tail leading to sum rule violations and majority spins are completely unaffected.

- A simple ladder approximation, on the other hand, correctly exhibits all of the qualitative features expected on general grounds for \( n_\downarrow > 0 \), however there are quantitative inaccuracies and the approximation breaks down for \( n_\downarrow / n_\uparrow \) larger than \( \sim 0.02 \).

### 3.1 Analytic Results

#### 3.1.1 Sum Rules and High Frequency Tail

The RF spectrum, introduced in Sec. 2.1, obeys exact sum rules [53, 54] for the zeroth \((l = 0)\) and first \((\ell = 1)\) moments of the RF intensity \( \int d\omega \omega^l I_\sigma(\omega) \) which are valid for all values of \( a \) and \( a_{e,\sigma} \). In our units they take the form

\[
\int_{-\infty}^{\infty} d\omega I_\sigma(\omega) = n_\sigma, \tag{3.1}
\]

\[
\int_{-\infty}^{\infty} d\omega \omega I_\sigma(\omega) = \left( \frac{1}{a} - \frac{1}{a_{e,\sigma}} \right) \frac{C}{4\pi m}, \tag{3.2}
\]

where we’ve set \( 2\pi\gamma^2 \equiv 1 \) above and in Eq. (2.4) to make the formulas simpler. It might seem that the first moment sum rule (clock shift), which diverges as \( a_{e,\sigma} \to 0^- \), can be of no use when final state interactions are negligible. However, we find that this divergence is actually related to a universal high frequency tail in \( I_\sigma(\omega) \), and that this is a general feature of the response. To see this, we rewrite Eq. (2.4) as

\[
I_\sigma(\omega) = \sum_k \int_{-\infty}^{\infty} d\Omega A_\sigma(k, \Omega)n_F(\Omega)\delta(\Omega - \epsilon_k + \mu_\sigma + \omega). \tag{3.3}
\]

This immediately leads to the zeroth moment sum rule, using \( \int d\Omega A_\sigma(k, \Omega)n_F(\Omega) = n_\sigma(k) \) and \( \sum_k n_\sigma(k) = n_\sigma \).

We next analyze the large frequency behavior of \( I_\sigma(\omega) \). The \( \delta \)-function then contributes in one of three ways: either (a) \( \Omega \) is large and negative with \( \epsilon_k \) small, (b) \( \Omega \) small but \( \epsilon_k \) large, or (c) both \( |\Omega| \) and \( \epsilon_k \) large such that they are comparable in magnitude. We can eliminate case (a) by noting that the spectral function \( A_\sigma \) generally vanishes as \( \Omega \to -\infty \) in order to satisfy the sum rule \( \int_{-\infty}^{\infty} d\omega A_\sigma(\omega) = 1 \). By considering only particle-particle
scattering for large momentum in the previous chapter [46] that, in many cases of interest for dilute Fermi gases, it is case (c) that is the dominant contribution. We therefore find 

\[ I_\sigma(\omega \rightarrow \infty) \simeq \sum_k n_\sigma(k) \delta(2\epsilon_k - \omega). \]

Using Tan’s result [47] for the momentum distribution, 

\[ n_\sigma(k) \simeq C/k^4 \quad \text{for} \quad k \gg k_F \sigma, \]

we thus find that 

\[ I_\sigma(\omega \rightarrow \infty) \approx \frac{1}{4\pi^2} \frac{C}{\sqrt{m} \omega^{3/2}}, \quad (3.4) \]

where \( C \) is the contact. We emphasize that the form of this result is independent of the phase (normal or superfluid) of the Fermi gas, though the value of \( C \) does depend on the phase. (This tail is absent only for the noninteracting gas for which \( C \equiv 0 \).) Note that this high frequency tail arises from short-distance physics in any Fermi gas, and is crucial for enforcing the divergent clock shift for \( a_{e,\sigma} = 0 \).

We finally note that, in the event that \( a_{e,\sigma} \neq 0 \) but small, we do expect a crossover from the above result to one in which the frequency dependence is \( \omega^{-5/2} \), and that this crossover occurs at an energy \( \omega \simeq 1/ma_{e,\sigma}^2 \). Such a crossover is consistent with, for example, the exact solution in the Bose limit by Chin and Julienne [70]. In fact, using the operator product expansion it has been shown [71] that this crossover does, indeed, exist. In this case, we restrict our result to \( \epsilon_{F,\sigma} \ll \omega \ll 1/ma_{e,\sigma}^2 \ll 1/mr_0^2 \), where \( r_0 \) is the range of the interatomic potential.

### 3.1.2 BCS mean field theory

In the study of many-body systems, various phases are often directly identified by characteristic low-energy singularities in measurable quantities, such as the discontinuity at \( k_F \) in
the momentum distribution of a Fermi liquid, or the square root singularity in the density of states of a s-wave superconductor at $T = 0$. Here we ask if any such singularity exists in the RF signal. We will first investigate the result from mean field theory. Using Eq. (2.4) with the BCS spectral function Eq. (2.8), we obtain, at zero temperature,

$$ I_{MF}(\omega) = \sum_k v_k^2 \delta(\xi_k - \omega + E_k) \theta(\omega - \xi_k). $$

(3.5)

Physically, we interpret the RF spectrum as pair breaking of atoms by creating holes at energy $\xi_k - \omega$. Since the single particle spectral function is sharply peaked at $-E_k$, only one momentum $k_0$ contributes to the integral. After manipulating the $\delta$-function we obtain

$$ I_{MF}(\omega) = \frac{m k_0(\omega)}{4\pi^2} \frac{v_{k_0}^2}{u_{k_0}^2}, $$

(3.6)

where $k_0(\omega)$ is defined by $\xi_{k_0}(\omega) - \omega + E_{k_0}(\omega) \equiv 0$. We find that the threshold of the spectrum occurs when $k = 0$: $\omega = E_0 + \xi_0 = \sqrt{\mu^2 + \Delta_0^2} - \mu$. We also find that there are no other singularities in the spectrum, other than the large-frequency tail

$$ I_{MF}(\omega) \to \frac{1}{4\pi^2 \sqrt{m}} \frac{C_{MF}}{\omega^{3/2}} $$

(3.7)

where $C_{MF} = m^2 \Delta_0^2$. As shown in the last chapter, this is a small correction to the true leading term of the contact coming from Fermi liquid corrections of short-range correlations.

### 3.1.3 Fermi Liquid Singularity

In the remainder of this chapter we focus on the normal (i.e., non-superfluid) ground state of the highly polarized Fermi gas. Thus our results are relevant, e.g., to the unitary gas which has been predicted to be a normal Fermi liquid for $x = n_{\downarrow}/n_{\uparrow} < 0.4$, based on QMC simulations [64]. (Our general results apply equally well to the dilute repulsive gas of Galitskii [40], which is yet to be realized in the laboratory.)

For a Landau Fermi liquid the spectral function is of the form

$$ A(k, \omega) \simeq Z \delta \left( \omega - \frac{k_F}{m^*}(k - k_F) \right) + A^{inc}(k, \omega) $$

(3.8)

close to the Fermi surface ($k \simeq k_F, \omega \simeq 0$). The subscript $\sigma$ is dropped for simplicity. The first “coherent” term gives the quasiparticle pole in the Green’s function with quasiparticle weight $Z$ and effective mass $m^*$, which are calculated in the usual way, by $Z = 1/[1 - \partial \Sigma'/\partial \omega]$ and $m/m^* = Z [1 + \partial \Sigma'/\partial \epsilon_k]$ evaluated at the Fermi surface: ($k = k_F, \omega = 0$). $k_F$ is unshifted from its bare value as required by Luttinger’s theorem [40]. The second non-singular term is the “incoherent” part of the spectral function.

The singular contribution to $I(\omega)$ is obtained by substituting the coherent term in
Eq. (3.8) into Eq. (2.4) and using $f(\epsilon) = \Theta(-\epsilon)$ at $T = 0$. We convert the $k$-sum to an integral over $\epsilon_k$ and write the quasiparticle dispersion as $k_F(k - k_F)/m^* \simeq (k^2 - k_F^2)2m^* = (\epsilon_k - \epsilon_F)m/m^*$. Considering $m^* > m$, we find a peak which grows like a square root in $\omega$, with a width equal to $(1 - m/m^*)\epsilon_F$, and then a discontinuous drop. This is then added to the smooth contribution from the incoherent piece. This is illustrated later in the thesis with dashed lines. The location of the discontinuity $\omega^*$ and the size of the jump $\Delta I$ are thus given by

$$\omega^*_\sigma = \epsilon_{F\sigma} - \mu_\sigma; \quad \Delta I_\sigma = \frac{Z_\sigma N(\epsilon_{F\sigma})}{1 - m/m^*_\sigma},$$

where $N(\epsilon_{F\sigma})$ is the density of states at the Fermi energy. We note here that the noninteracting limit, corresponding to $m^* \simeq m$ and $Z \to 1$, results in a singular contribution to $I(\omega)$ at $\omega^* \to 0$ in such a way that the total weight is $N(\epsilon_{F\sigma})$, while the incoherent contribution vanishes.

### 3.2 Diagrammatic Approaches in Spin-Imbalanced Phase

The form of the Fermi surface singularity and the high energy tail in the RF intensity have been elucidated above on general grounds. Calculating the detailed lineshape $I_{rf}(\omega)$, however, necessarily requires approximations to be made for a strongly interacting Fermi system. Here we describe diagrammatic calculations for the highly imbalanced normal gas at unitarity $a_s \to \infty$, highlighting the successes and limitations of two approximation schemes. All such calculations of the self energy on the Matsubara axis use the diagrammatic formulation we derived in the previous chapter, and so we will not repeat the formulas.

#### 3.2.1 Self-consistent method

Let us first discuss a simple self-consistent approximation [54], motivated by an analysis that reproduces the essentially exact result [29] of a single ↓ spin ($n_{\downarrow} = 0$ limit) interacting with a Fermi sea of ↑ fermions [64]. We will show that this scheme has serious qualitative problems for $n_{\downarrow} > 0$ and analyze why this is the case. In this approximation, the internal Green’s function lines used to calculate $\Gamma$ and $\Sigma$ are the free-particle Green’s functions in form, but with a renormalized chemical potential. A self-consistency condition is then imposed so that $\mu_{\downarrow} = \epsilon_{F\downarrow} + \Sigma'_{\downarrow}(k_{F\downarrow}, 0; \mu_{\downarrow})$, where $\Sigma'_{\downarrow}$ itself depends on $\mu_{\downarrow}$ [29, 69], thus ensuring that there is a pole in $G$ at the Fermi surface. For the single minority spin limit ($k_{F\downarrow} \to 0$), this reproduces the result $\mu_{\downarrow}(n_{\downarrow} = 0) = -E_b \simeq -0.6\epsilon_{F\downarrow}$.

This approximation for $n_{\downarrow} > 0$ implies the use of a negative $\mu_{\downarrow}$ in the bare Green’s function used in $\Gamma$ and $\Sigma$. As a result, one misses all effects of finite $n_{\downarrow}$ occupancy “inside” the calculation. We can then analytically see that $\text{Im}\Gamma(Q, \Omega < 0) \equiv 0$. Let us rewrite
Figure 3.2: Momentum distribution $n_k$ (left) and RF spectrum $I_\uparrow(\omega)$ (right) of a unitary Fermi gas with $n_\downarrow/n_\uparrow = 0.01$ calculated within the self consistent approximation. The majority $n_{k\uparrow}$ is the free Fermi spectrum, while $n_{k\downarrow}$ has an interaction-suppressed value, but is zero for $k > k_F$. The majority spectrum $I_\uparrow$ (left, red) is a delta function with weight $n_\uparrow$. The minority (right, blue) spectrum has a discontinuity and a shift due to interactions, but no high frequency tail. The dashed line indicates the jump.

$$\Gamma^{-1}(Q, \Omega) \equiv 1/g - L(Q, \Omega),$$

where $L$ is given by

$$L(Q, \Omega) = \sum_p \left[ \frac{1}{2\varepsilon_p} + \frac{1 - n_F(\xi_{p,\downarrow}) - n_F(\xi_{p-Q,\downarrow})}{\Omega - \xi_{p-Q,\downarrow} - \xi_{p,\uparrow}} \right]. \quad (3.10)$$

The second term describes two-particle scattering in the medium of the unitary gas. As long as $\mu_\downarrow < 0$, however, the second Fermi function is zero. Furthermore, the resulting $\delta$-function $\delta(\Omega - \xi_{p-Q,\downarrow} - \xi_{p,\uparrow})$ requires $\xi_{p,\uparrow} < 0$, and therefore the occupation factor is $1 - n_F(\xi_{p,\uparrow}) = \Theta(\xi_{p,\uparrow}) = 0$ at $T = 0$. The imaginary part of $L$ (and therefore $\Gamma$) is then zero for all $\Omega < 0$, and therefore the minority scattering is never incorporated.

Looking to the imaginary part of the self energy, Eq. (2.12), we see that the integration for $\omega < 0$ requires negative energy values of $\text{Im}\Gamma$, which means that $A^{\text{inc}}_\downarrow(k, \omega < 0) \equiv 0$ and $A_\downarrow(k, \omega < 0)$ has only a pole for each $k$ with a weight $Z_{k,\downarrow} < 1$. Thus, $n_\downarrow(k) = Z_k \Theta(k_{F\downarrow} - k)$ and consequently both the sum rules $\sum_k n_\downarrow(k) = ZN_\downarrow < N_\downarrow$ and $\int d\omega I_\downarrow(\omega)$ are violated in a qualitative way. In addition, in the absence of any incoherent spectral weight for $\omega < 0$, one also misses both the universal $k^{-4}$ tail in $n_\downarrow(k)$ and the $\omega^{-3/2}$ tail in the RF spectrum (see Fig. 3.2). The first moment of $I_\downarrow(\omega)$ is then finite, instead of diverging as it should due to Eq. (3.2).

Finally, for the majority self energy $\Sigma_\uparrow$, the occupation factors in Eq. (2.12) are identically zero, meaning the majority spins are completely unaffected by interactions, which is clearly unphysical for finite minority density. The majority ($\uparrow$) RF spectrum is thus a
\(\delta\)-function, a result that is at odds with all available experiments. Clearly, this approximation fails to provide a reasonable description of RF spectra of highly imbalanced gases, despite its success in obtaining reasonable numerical estimates for \(\mu_\downarrow\). All of the problems here arise from the fact that propagators with renormalized \(\mu_\downarrow < 0\) are used without taking into the shifts in the \(\downarrow\) particle dispersion.

### 3.2.2 Large-\(\mathcal{N}\) Calculation

This suggests that it may be physically more sensible to do the simplest calculation without any attempts at partial self-consistency, i.e., evaluate all diagrams with free-particle propagators with \(\mu_\sigma = \epsilon_{F\sigma}\) for the self energy, Eq. (2.12). This leads to equations which are identical with the first order term in the \(1/\mathcal{N}\) approximation [63] with \(\mathcal{N} = 1\) at the end. Now, in contrast to the previous approximation, the vertex \(\text{Im}\Gamma\) has structure even for \(\Omega < 0\), as illustrated in Fig. 2.6. This leads to \(n(k)\) and \(I(\omega)\) with universal tails for both spins, as we describe below.

The finite weight in \(\text{Im}\Gamma\) for \(\Omega < 0\) appears precisely due to the Fermi function for minority atoms in \(L''\) becoming nonzero, in contrast to the previous section. The physical meaning of this is that once a finite density of minority spins is allowed in the calculation, there is phase space available for two-particle (hole) scattering, but only at low energies determined by energetics, due to being at \(T = 0\). The threshold for nonzero weight then becomes \(\Omega_0(Q) = \epsilon_Q/2 - \epsilon_{F\uparrow} - \epsilon_{F\downarrow}\), which can be negative. We note that finite temperature would result in finite, but exponentially suppressed, weight below this threshold due to the occupation factors in Eq. (3.10). This therefore doesn’t change our results qualitatively.

This therefore leads to a nonzero \(\text{Im}\Sigma\), since, from the previous section, negative energy values of \(\text{Im}\Gamma\) are required for its evaluation. The spectral function is therefore qualitatively different from the previous section (which is only a \(\delta\)-function for \(\omega < 0\)), but captures generally correct features. As noted in the previous chapter, it contains an incoherent branch at large \(k\) whose peak increases asymptotically to \(-\epsilon_k\) as \(k\) increases [46]. We also note the quasiparticle pole at \(k_{F\downarrow}\) due to the Fermi liquid nature of the gas.

Our numerical results for the momentum distributions and RF spectra for the unitary Fermi gas with polarization \(x = 0.01\) are shown in Fig. 3.3. Both majority and minority spectra show jump discontinuities and high momentum and high frequency tails. The spin-independent \(k^{-4}\) and \(\omega^{-3/2}\) behavior tails are also observed. In comparing with the results of the previous section in Fig. 3.2 and the current approximation in Fig. 3.3, there is no doubt that the latter provides a far better qualitative description.

Despite these qualitative successes, however, it must be emphasized that the simple ladder approximation is not quantitatively accurate insofar as the calculated chemical potentials (e.g., \(\mu_\downarrow = \epsilon_{F\downarrow} + \Sigma_\downarrow'(k_{F\downarrow}, 0; \epsilon_{F\downarrow})\)) and RF sum rules are concerned. In particular, we find that in the single spin limit \(\mu_\downarrow(n_\downarrow = 0) \simeq -0.9\epsilon_{F\downarrow}\), as compared with the exact
result of $-0.6\epsilon_{F\uparrow}$. Moreover, we have found that the simple ladder approximation leads to a negative compressibility a density ratio above $x \sim 0.02$ clearly signaling the limitations of the approximation.

### 3.3 Comparison With Experiment

In order to compare with experiments, it is necessary to note that they are performed at finite (but low) temperature, final-state scattering length $a_{e,\sigma}$, and in an inhomogeneous trap. Our exact results, however, still allow us to analyze RF spectra. Tomographically reconstructed data is now available which minimizes trap effects and allows us to focus on specific regions of the cloud, namely, the balanced superfluid on the inside and the polarized normal region on the outside.

Let us begin with the universal high frequency tail. Finite temperature results in exponential corrections in the particle-particle vertex, and therefore in the spectral function, and in the tail of the RF spectrum. So, provided the temperature is low enough we can still proceed. The high frequency tail is certainly seen in experiments in $^6$Li [44, 45] and recently, a direct test of the high frequency and momentum tails [39] confirms the predictions explicitly in $^{40}$K.

The jump discontinuity in the $T = 0$ RF signal for a normal Fermi liquid will of course be broadened by finite temperature and experimental resolution. The best we can expect

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3Final state interactions are minimized by choosing good hyperfine states that are occupied initially in the trap; $(1/ma_{e,\sigma}^2)/\epsilon_{F\uparrow} = 1/(k_{F\uparrow}a_{e,\sigma})^2 \simeq 40$, and therefore as noted in the previous section this gives a window of energy for a fit.
then is to see a peak at, or very close to, the location of the discontinuity. The equation of state from QMC calculations \cite{64} is

\[
E = \frac{3}{5} N_\uparrow \epsilon_{F\uparrow} \left( 1 - A_0 x + \frac{m}{m_0^*} x^{5/3} + F x^2 \right)
\]

where \( x = n_\downarrow / n_\uparrow \), \( E_b = 3 A_0 \epsilon_{F\downarrow} / 5 \) is the binding energy and \( m_0^* \) the effective mass of a single \( \downarrow \) spin, and \( F \) a Fermi-liquid correction. We use \( m_0^* \) here since \( m^* \) is in general \( x \)-dependent. After finding \( \mu_\downarrow \), eq. (3.9) predicts the position of the Fermi liquid discontinuity to be

\[
\frac{\omega^*_\downarrow}{\epsilon_{F\downarrow}} = \frac{3}{5} A_0 - \left( 1 - \frac{m}{m_0} \right) x^{2/3} - \frac{6}{5} F x.
\]

This is exactly the expression used for the peak position by Schirotszek et al. \cite{45}. For the majority spins, with \( m^* \simeq m \), the peak will be at \( \omega^*_\uparrow / \epsilon_{F\uparrow} = 2 A_0 x / 5 + F x^2 / 5 \), which is slightly shifted from zero.
Chapter 4
Spectral Function in the Superfluid State

As mentioned in chapter 2, the measurement of the single particle spectral function, via angle-resolved RF spectroscopy is a particularly exciting prospect [42], as one can gain information about the spectrum and dynamics of single-particle excitations. Recent experiments [21, 72] have been able to study with detail the lineshape of $A(k, \omega)$ at finite temperature in order to study the low energy spectrum. Motivated by this capability, we turn the superfluid state at zero temperature, in order to address the question of whether sharp quasiparticles exist here across the BEC-BCS crossover and what their dispersion looks like.

Quite generally, quasiparticles are very important concepts in condensed matter physics, allowing one to describe the low energy excitations as a set of weakly interacting ones, even though the “bare” particles in the system may be subject to arbitrarily strong interactions. For normal Fermi liquids, the Landau quasiparticles are sharp (i.e., well-defined in energy) fermionic excitations. These gapless excitations live on the Fermi surface, with a Fermi wavevector $k_F$ that is unrenormalized by interactions (Luttinger’s theorem [73]).

For a paired superfluid, the BCS theory predicts the existence of sharp Bogoliubov quasiparticles, which are gapped fermionic excitations. Since weak coupling BCS theory is essentially a Hartree-Fock theory, the Bogoliubov excitations are sharp, and, in fact, the lowest energy excitations correspond to $k = k_F$. However, there is no Luttinger’s theorem for a state with superfluid long range order [74, 75], thus there is no reason for the minimum gap to correspond to $k = k_F$, determined by the density and independent of interactions. In fact, we will see a clear example of this general result below.

An even more important question, on which there has been some debate in the recent literature, is the following. Are there sharp, well-defined Bogoliubov quasiparticles across the entire BEC-BCS crossover or do the effects of strong interactions destroy the sharp excitations outside the weak-coupling BCS limit?
The dispersion of the gapped fermionic excitations in the superfluid state has been inferred from (angle-integrated) RF spectroscopy [44], and been determined from $T = 0$ QMC [76] calculations that compute energies of excited states. However, neither of these techniques directly addresses the question of whether these excitations are sharp. Unfortunately, angle-resolved RF experiments, which can in principle address this question, have at the present too poor an energy resolution (approximately 0.25 times the Fermi energy) to shed light on the issue. Diagrammatic calculations [65, 77] are also not conclusive on this question. In part, the problem arises because many calculations, such as the Luttinger-Ward approach of Ref. [65], work in Matsubara frequencies and then use approximate methods to continue to real frequencies using, e.g., the maximum entropy method. Sharp features in spectral functions cannot be resolved in such analytic continuation schemes. Using a particular approximation, the authors of Ref. [78] concluded unequivocally that the inclusion of fluctuations destroys sharp quasiparticles in the strongly interacting regime.

We will use here a real frequency $T = 0$ approach that does not suffer from the above limitations and can see sharp quasiparticles, if they exist. We will conclude that they do exist across the entire BEC-BCS crossover, understanding in detail why the approximation of Ref. [78] failed to see them.

We summarize our main results as follows:

- We present a general argument for sharp Bogoliubov quasiparticles using phase space considerations for the interaction of low energy fermionic excitations with the low energy collective modes (phonons) which dominates their decay near the bottom of the dispersion.
- We find that sharp quasiparticle peaks do exist in the system from weak coupling through unitarity and into the BEC limit.
- We present the simplest calculation of the low-energy spectral function which illustrates these features, namely, the Gaussian fluctuation approximation. This theory has been used extensively [13, 16, 79] to calculate the equation of state in the crossover. It has been shown to have good agreement with QMC at unitarity as well as in the BEC limit and is asymptotically exact in the weak coupling limit. We also discuss a closely related large-$N$ approximation scheme using a Sp$(2N)$ symmetric theory of $N$ species of two-component fermions [61, 62].
- We show that the fluctuation corrections, in addition to lowering the single particle gap as expected, also lead to an interesting renormalization of the dispersion so that the location of the minimum of the Bogoliubov spectrum is shifted away from $k_\mu = \sqrt{2m\mu}$, as predicted by mean field theory, to a much larger $k_{\min}$.

To make contact with earlier work, we use the following parameterization of the single
particle dispersion, inspired by mean field theory [12],

\[ \tilde{E}_k = \sqrt{\left( \frac{k^2}{2m^*} - \mu + U \right)^2 + \Delta^2}, \]  

(4.1)

Here \( \Delta \) is the gap, the self-energy \( U \) provides a shift from the minimum wavevector \( k_{\text{min}} \) from the chemical potential, and \( m^* \) is an effective mass. The minimum of the dispersion is found by setting \( \frac{k_{\text{min}}^2}{2m^*} - \mu + U = 0 \). In mean field theory, \( U = 0 \) and \( m^* = m \) and the minimum is at \( k_{\mu} = \sqrt{2m\mu} \) when \( \mu > 0 \). It turns out that \( U \) is large and negative, leading to a strong renormalization of \( k_{\text{min}} \). Although the \( U \) value calculated at unitarity from the gaussian approximation theory is not in quantitative agreement with the QMC (see Tbl. 4.1 below), we nevertheless get a qualitative understanding of its sign and magnitude.

Finally, we note that calling \( U \) a “Hartree shift”, as is often done in the literature, is quite misleading. It is not proportional to the interaction times the density even in weak coupling and at unitarity the interaction is infinitely strong! Thus \( U \) is best thought of as a non-trivial self energy correction in the dispersion.

4.1 Green’s Function Formalism

We start our discussion by writing down the single particle Green’s function, a matrix in the field operators \( \psi_\sigma(x, t) \). Using the row spinor \( \Psi^\dagger(x, t) \equiv \left( \psi^\dagger_\uparrow(x, t), \psi_\downarrow(x, t) \right) \) we can write the Green’s function in a translationally invariant system in equilibrium as

\[ \hat{G}(x - x', t - t') = -\left( T \begin{pmatrix} \psi_\uparrow(x, t)\psi^\dagger_\uparrow(x', t') & \psi_\uparrow(x, t)\psi_\downarrow(x', t') \\ \psi_\downarrow(x, t)\psi^\dagger_\downarrow(x', t') & \psi_\downarrow(x, t)\psi^\dagger_\uparrow(x', t') \end{pmatrix} \right). \]  

(4.2)

In momentum and Matsubara frequency, the Green’s function is

\[ \hat{G}(k, ik_n) = \begin{pmatrix} G(k, ik_n) & F(k, ik_n) \\ F(k, ik_n) & -G(-k, -ik_n) \end{pmatrix}, \]  

(4.3)

where \( ik_n = i(2n + 1)\pi/\beta \) are the Matsubara frequencies and we’ve exploited the spin symmetry. Dyson’s equation defines the self energy

\[ \hat{G}^{-1}(k, ik_n) = (\hat{G}^0)^{-1}(k, ik_n) - \hat{\Sigma}(k, ik_n), \]  

(4.4)

where the “free” Green’s function here is the mean field solution,

\[ \hat{G}^0(k, ik_n) = \frac{1}{(ik_n)^2 - E_k^2} \begin{pmatrix} ik_n + \xi_k & -\Delta_0 \\ -\Delta_0 & ik_n - \xi_k \end{pmatrix}. \]  

(4.5)

We use the time reversal invariance of the system, which sets to zero the component of the self energy matrix which depends on the Pauli matrix \( \hat{\sigma}_y \) (See argument by D. Scalapino,
The self energy then takes the form
\[
\hat{\Sigma}(k, ik_n) = \begin{pmatrix} \Sigma(k, ik_n) & S(k, ik_n) \\ S(k, ik_n) & -\Sigma(-k, -ik_n) \end{pmatrix}.
\] (4.6)

Note that a direct consequence of this argument is that the anomalous Green’s functions are equal, \( F = \overline{F} \), and symmetric in the arguments, \( F(k, ik_n) = F(-k, -ik_n) \), which leads to \( F(k, -\omega) = F^*(k, \omega) \) on the real frequency axis. The spectral functions are then taken from the first and second elements of \( \hat{G} \) after analytic continuation
\[
A(k, \omega) = -\frac{1}{\pi} \text{Im} \ G(k, \omega + i0^+), \quad B(k, \omega) = -\frac{1}{\pi} \text{Im} \ F(k, \omega + i0^+),
\] (4.7)
where we intentionally neglect the carets to signify that they are scalars. To allow for the possibility of sharp \( \delta \)-functions in the spectrum at energy \( E_g(k) \), we note that the Green’s function
\[
G(k, \omega) = \frac{\omega + \xi_k + \Sigma^*(\omega)}{\text{det} \ \hat{G}^{-1}(k, \omega)}
\] (4.8)
must have a pole at \( \omega = E_g(k) \), or \( \text{det} \ \hat{G}^{-1}(k, E_g(k)) \equiv 0 \). Note that, in this case, the self energy is real, and we see that \( \text{det} \ \hat{G}^{-1}(k, E_g(k)) \) symmetric in the sign of \( E_g(k) \), and so we define \( E_g(k) > 0 \) and not explicitly show solutions for \( -E_g(k) \). Writing the general forms for \( A \) and \( B \) in the vicinity of the quasiparticle dispersion (namely, \( k \approx k_{\text{min}} \) and \( \omega \approx E_g(k) \)), which include both the coherent weight associated with the quasiparticles and the incoherent parts of the decay, we have
\[
A(k, \omega) = Z_k^+ \delta(\omega - E_g(k)) + Z_k^- \delta(\omega + E_g(k)) + A_{\text{inc}}(k, \omega)
\] (4.9)
and
\[
B(k, \omega) = -Y_k \delta(\omega - E_g(k)) + Y_k \delta(\omega + E_g(k)) + B_{\text{inc}}(k, \omega)
\] (4.10)
where the quasiparticle weight for \( \omega > 0 \) is given by
\[
\frac{1}{Z_k^+} = \left. \frac{\partial G^{-1}(k, \omega)}{\partial \omega} \right|_{\omega = E_g(k)}
\] (4.11)
and the weights \( Z_k^- \) and \( Y_k \) are related to \( Z_k^+ \) by
\[
Z_k^- = \frac{E_g(k) - \xi_k - \Sigma(k, E_g(k))}{E_g(k) + \xi_k + \Sigma(k, -E_g(k))} Z_k^+, \quad Y_k = \frac{\Delta_0 - S_k(E_g(k))}{E_g(k) + \xi_k + \Sigma(k, -E_g(k))} Z_k^+.
\] (4.12)
Note that in the gauge we have considered, $Y_k > 0$. Finally, the minimum of the dispersion is determined by setting the velocity

$$v_k = \frac{\partial E_g(k)}{\partial k}$$

(4.13)
to zero. This is as far as an exact analysis can take us. In the mean field theory, the self energy is zero, meaning the incoherent weights vanish, and

$$Z^+_k = u_k^2, \quad Z^-_k = v_k^2, \quad Y_k = u_kv_k.$$ 

(4.14)

Using this general formalism, we now turn to a discussion of the low energy form of the interaction.

### 4.2 Low Energy Effective Theory

We will now focus on the low energy physics of the spectral function, and provide a general self consistent argument in favor of low energy quasiparticles with dispersion $E_g(k)$ by determining the leading order behavior of the Green’s function. If we restrict ourselves to the bottom of the fermionic dispersion, the only decay processes available to excitations which are infinitesimally above the gap are the emission of long-wavelength phonons. To construct the diagrams, then, we use double arrow notation to draw the full Green’s function [40]

$$\hat{G}(k, ik_n) = \begin{pmatrix} \square & \square \\ \square & \square \end{pmatrix},$$

(4.15)

which is equivalent to Eq. (4.3). Here, the arrows going right indicate $k, ik_n, \uparrow$, and those to the left indicate $-k, -ik_n, \downarrow$. The effective interaction has the same notation, only with wavy lines and no spins. In arbitrary diagrams, one uses the vertex rules to determine the arrow directions. Two Green’s function arrows come to a vertex and a fluctuation arrow flows out (or vice-versa by reversing all arrows, $k, ik_n$, and spins). The decay, then, from the imaginary part of the self energy, is given by a single vertex as shown in the diagram of Fig. 4.1. The first two elements of the full Green’s function are written as

$$G(k, \omega) = \frac{Z^+_k}{\omega^+ - E_g(k)} + \frac{Z^-_k}{\omega^+ + E_g(k)} + G^{inc}(k, \omega)$$

(4.16)

$$F(k, \omega) = -\frac{Y_k}{\omega^+ - E_g(k)} + \frac{Y_k}{\omega^+ + E_g(k)} + F^{inc}(k, \omega)$$

(4.17)

where $\omega^+ \equiv \omega + i0^+$ and the imaginary parts are given by Eqs. (4.9) and (4.10). The effective interaction, which also serves as the phonon propagator, has the general form for
\[ k + q, \omega - E_q \]

\[ k, \omega \]

\[ -q, -E_q \]

Figure 4.1: Feynman diagram for the low energy part of the imaginary part of the self energy $\hat{\Sigma}$. Figure contains one vertex consisting of the renormalized effective interaction $\hat{\Gamma}_{11}$ as double wavy line and Green’s function $\hat{G}_{22}$ as double straight line.

low energies (See Sec. 24.3 of Ref. [40])

\[ \hat{\Gamma}_{11}(q) \equiv -\frac{\zeta}{(\omega^+)^2 - c_s^2 q^2} + \hat{\Gamma}_{11}^{\text{inc}}(q), \quad \hat{\Gamma}_{12}(q) \equiv -\frac{\zeta}{(\omega^+)^2 - c_s^2 q^2} + \hat{\Gamma}_{12}^{\text{inc}}(q), \quad (4.18) \]

where $\zeta$ is a positive constant. We make a brief note that $\hat{\Gamma}$ is actually the negative of the phonon propagator, as one can verify by expanding the partition function. The speed of sound is $c_s$. We point out that the values of $\zeta$ and $c_s$ depend on the use of approximations, but the form of the phonon propagator here is a general property of neutral superfluid systems, and in principal one can obtain the exact propagator which contains the real values. We take advantage of this generality by using $\zeta$ and $c_s$ as parameters.

The imaginary part of Fig. 4.1 is obtained by standard diagrammatic theory, keeping only the most singular parts of $\hat{G}$ and $\hat{\Gamma}$, since all other pieces will be subleading. We obtain

\[ \text{Im } \Sigma(k, \omega) = -\pi \sum_q \left[ Z^-(q) Z^+ \delta(\omega + E_g(q - k) + \Omega_0(q)) - Z^+(q) Z^- \delta(\omega - E_g(q - k) - \Omega_0(q)) \right] \quad (4.19) \]

and

\[ \text{Im } S(k, \omega) = -\pi \sum_q Y_T(q) Y \delta(\omega - E_g(q - k) - \Omega_0(q)) \quad (4.20) \]

where $\Omega_0(q) \simeq c_s q$ is the collective mode energy and $Z^\pm_T = \mp \zeta / q$, $Y_T = \zeta / q$ are its residues. The physics of the above expressions comes from considering a positive (negative) frequency excitation which emits a phonon to decay to a quasiparticle state with energy $E_g$ and weight $Z^-$ ($Z^+$). The reason that the weights involved are of the opposite sign is due to the matrix structure - a $\uparrow$ spin interacts with a $\downarrow$ hole, and vice-versa.

Now, by making an expansion in small values of $\omega - \Delta$, we can expand the real and imag-
inary parts of $\hat{\Sigma}$ and eventually find the behavior of $G$. As shown in Sec. 4.7, each element of the imaginary part of the self energy is linear in frequency according to $\hat{\Sigma}_{ij}(k, \omega) \sim (\omega - \Delta)$. Of course, the real parts of the self energy are not calculable with Fig. 4.1, however, we can still determine the leading order behavior using the Kramers-Kronig relations for each element by

$$\text{Re } \hat{\Sigma}(k, \omega) = -\frac{1}{\pi} \mathrm{P} \int_{-\infty}^{\infty} dz \frac{\text{Im } \hat{\Sigma}(k, \omega)}{\omega - z}. \quad (4.21)$$

We subsequently find that each element acquires a dependence of the form $(\omega - \Delta) \ln(\omega - \Delta)$ with a subleading linear dependence. Even though one might conclude, as in Ref. [78], that $Z^+$ must vanish, we point out that, for the inverse Green’s function $G^{-1}$, these logarithmic dependences actually cancel out in Eq. (4.11), as shown in Sec. 4.7. Furthermore, the spectral function

$$A(k, \omega) = \frac{1}{\pi} \frac{\text{Im } G^{-1}(k, \omega)}{[\text{Re } G^{-1}(k, \omega)]^2 + [\text{Im } G^{-1}(k, \omega)]^2} \quad (4.22)$$

has the leading order dependence on energy $(\omega - \Delta) \ln(\omega - \Delta) \to 0$ as $\omega \to \Delta^+$. We therefore do in fact obtain sharp $\delta$-functions in the fermionic spectra. This then provides a self-consistent argument that quasiparticles exist in the system, and we next turn to the results of the gaussian approximation which is the simplest calculation that exhibits all the above general features.

We make a final note that this analysis applies only to the bottom of the dispersion when $Z^+_{k}$ is well-defined. As noted in Ref. [65], however, one can make an argument for the width of the sharp region in the spectral function by considering the group velocity, Eq. (4.13), of the spectrum, and comparing it to the speed of sound $c_s$. In the weak coupling limit, for example, $c_s = v_F/\sqrt{3}$ and $|\partial_k E_g(k)| < c_s$ only in an exponentially small region.

4.3 Gaussian Approximation

To perform the gaussian approximation, we start with the functional integral representation of the partition function $Z$. Expressed as a coherent state path integral over the Grassmann fields $\psi_\sigma$ and $\bar{\psi}_\sigma$, the partition function and action $S$ take the form

$$Z = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S[\bar{\psi},\psi]}, \quad S[\bar{\psi},\psi] = \int d^4x \left( \bar{\psi}_\sigma \partial_\tau \psi_\sigma - H[\bar{\psi},\psi] \right). \quad (4.23)$$

We will use the Hubbard-Stratonovich transformation to decompose the quartic interaction term in the pairing channel, giving the new representation of the partition function

$$Z = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \mathcal{D} \Delta^\ast \mathcal{D} \Delta e^{-S[\bar{\psi},\psi,\Delta^\ast,\Delta]}, \quad (4.24)$$

44
where the new action is
\[
S[\overline{\psi}, \psi, \Delta^*, \Delta] = \int d^4x \left[ \frac{|\Delta(x)|^2}{g_\Lambda} - \int d^4x' \overline{\Psi}_\alpha(x) \hat{G}^{-1}_{\alpha,\beta}(x,x') \Psi_\beta(x') \right]
\]  
(4.25)

and we’ve defined the Nambu spinor \( \overline{\Psi} \equiv (\overline{\psi}_\uparrow, \overline{\psi}_\downarrow) \) and identified the inverse Nambu-Gorkov Green’s function
\[
\hat{G}^{-1} = \delta(x - x') \begin{pmatrix}
-\partial_x + \frac{\nabla^2}{2m} + \mu_\uparrow & \Delta(x) \\
\Delta^*(x) & -\partial_x - \frac{\nabla^2}{2m} - \mu_\downarrow
\end{pmatrix}.
\]  
(4.26)

We can now integrate out the fermions to obtain the effective action
\[
Z = \int \mathcal{D}\Delta^* \mathcal{D}\Delta e^{-S_{\text{eff}}[\Delta^*, \Delta]}, \quad S_{\text{eff}}[\Delta^*, \Delta] = \int d^4x \frac{|\Delta(x)|^2}{g_\Lambda} - \text{Tr} \ln \hat{G}^{-1},
\]  
(4.27)

where the trace above (with a capital “T”) includes both the Nambu trace and a trace over either space-time or momentum-frequency. This is as far as exact manipulations can take us, and we must now use approximations. For example, the BCS-Leggett mean field theory is obtained from a saddle point approximation, where the mean field partition function becomes \( Z_0 = \exp(-S_{\text{eff}}[\Delta^*_0, \Delta_0]) \), where \( \Delta_0 \) is obtained from the gap equation, \( \delta S_{\text{eff}} / \delta \Delta \equiv 0 \), or, equivalently, Eq. (1.20) with \( \epsilon_F \) replaced with \( \mu \). Again, the number equation is obtained from the thermodynamic potential, \( \Omega_0 = -T \ln Z_0 \).

To obtain the propagator of the Goldstone excitations of the system, we expand in gaussian fluctuations \([13, 16, 79]\) of the order parameter around the mean field solution, defining \( \Delta(x) \equiv \Delta_0 + \eta(x) \). We then obtain the fluctuation propagator from the action in the form
\[
S \simeq S_0 + \frac{1}{2} \sum_q \begin{pmatrix} \eta_q^* \\ \eta_{-q} \end{pmatrix} \hat{\Gamma}^{-1}(q) \begin{pmatrix} \eta_q \\ \eta_{-q}^* \end{pmatrix},
\]  
(4.28)

where
\[
\hat{\Gamma}^{-1}(q) = \begin{pmatrix} M(q) & L(q) \\ L(q) & M(-q) \end{pmatrix}
\]  
(4.29)

with elements
\[
M(Q) = -\frac{m}{4\pi a} + \sum_p \left[ \frac{1}{2\epsilon_p} + \frac{u_p^2 u_{p+Q}^2}{iQ_l - E_p - E_{p+Q}} - \frac{v_p^2 v_{p+Q}^2}{iQ_l + E_p + E_{p+Q}} \right],
\]  
(4.30)
\[
L(Q) = \sum_p u_p u_{p+Q} v_p v_{p+Q} \left[ \frac{1}{iQ_l + E_p + E_{p+Q}} - \frac{1}{iQ_l - E_p - E_{p+Q}} \right].
\]  
(4.31)
Figure 4.2: Feynman diagrams in the gaussian approximation contributing to the self energy. Top: the diagonal and off-diagonal self energy $\hat{\Sigma}_{11}$ and $\hat{\Sigma}_{12}$. Bottom: the diagonal and off-diagonal effective interaction $\hat{\Gamma}_{11}$ and $\hat{\Gamma}_{12}$. The single wavy line is the bare propagator for the interaction $g_\Lambda$ (actually, the negative of the propagator). The arrow conventions for $\hat{\Gamma}$ are the same as for $\hat{G}$. See the discussion surrounding Eq. 4.15 for the momentum labeling rules.
and
\[
\nu_q^2 = \frac{1}{2} \left( 1 + \frac{\xi_q}{E_q} \right), \quad \nu_q^2 = \frac{1}{2} \left( 1 - \frac{\xi_q}{E_q} \right)
\]
(4.32)
are the Bogoliubov functions from the mean field solution. The class of diagrams we are considering is illustrated by Fig. 4.2, where the solid lines represent mean field quasiparticles, which now scatter off one another. The effective interaction diagrams look like the random phase approximation [13], where all possible vertices are used. One can verify that the small \( Q, iQ_l \rightarrow \omega + i0^+ \) limit of \( \hat{\Gamma} \) we have here indeed has the general form in Eq. (4.18). The self energy becomes, again using standard diagrammatic theory,
\[
\Sigma(k, ik_n) = -\frac{1}{\beta} \sum_{q,l} \hat{\Gamma}_{11}(q) G^0(q - k),
\]
(4.33)
\[
S(k, ik_n) = \frac{1}{\beta} \sum_{q,l} \hat{\Gamma}_{12}(q) F^0(q - k).
\]
(4.34)

We comment briefly on the signs of the above expressions. Note that the sign of \( \Sigma \) can be confirmed by forcing \( A > 0 \), but the sign of \( S \) cannot, since \( \Sigma \) always dominates over \( S \) when forcing \( A > 0 \) and there is no corresponding inequality for \( B \). However, by explicitly expanding the partition function, Eqs. (4.24) and (4.25), in small fluctuations of \( \Delta(x) \), one can see that the sign is, in fact, correct. After performing the Matsubara sums and the zero temperature limit, the imaginary parts of the self energy become
\[
\text{Im } \Sigma(k, \omega) = -\varepsilon \sum_q \frac{1}{2} \left( 1 - \varepsilon \frac{\xi_q}{E_q} \right) \Theta(|\omega| - E_q) \text{Im } \hat{\Gamma}_{11}(q + k, \omega - \varepsilon E_q),
\]
(4.35)
\[
\text{Im } S(k, \omega) = \sum_q \nu_q \nu_q \Theta(|\omega| - E_q) \text{Im } \hat{\Gamma}_{12}(k + q, \omega - \varepsilon E_q),
\]
(4.36)
where we’ve defined a shorthand \( \varepsilon \equiv \text{sgn}(\omega) \) to compact the notation. Note that these are of the same form as the general expressions (4.19) and (4.20) with the fermionic weights replaced by the mean field \( \nu_k, \nu_k \) and \( \hat{\Gamma} \) with that of the gaussian theory. There are also occupation factors which are important for arbitrary \( (k, \omega) \). The real parts of the self energy are calculated numerically using the Kramers-Kronig relation, Eq. (4.21).

We can expect that including fluctuations around the mean field solution brings about a broad continuum of scattering weight \( A^{\text{inc}} \), reducing the weights \( Z^\pm, Y \) of the sharp peaks. This weight is constrained by the general sum rules (which, in the calculation, are satisfied to within a maximum of 0.001)
\[
\int_{-\infty}^{\infty} d\omega A(k, \omega) = 1, \quad \int_{-\infty}^{\infty} d\omega B(k, \omega) = 0, \quad \int_{-\infty}^{\infty} d\omega \omega B(k, \omega) = -\Delta_0.
\]
(4.37)
However, it is appropriate to mention that the scattering weight, while important for the
renormalization of the quasiparticle dispersion $E_g(k)$ and for calculating these sum rules, does not interest us otherwise. Since this is a nonselfconsistent calculation, there is no reason to believe that the dispersion we calculate will match the threshold to scattering and, in fact, does not. The scattering threshold in the gaussian calculation occurs at the mean field level, for example, at unitarity in Fig. 4.3 the threshold occurs when $k = k_\mu \simeq 0.63k_F$ and $\omega = \Delta_0 \simeq 0.58\epsilon_F$. One must then check that the pole occurs outside the scattering continuum in order for the quasiparticle weight $Z^+$ to be well-defined. We therefore focus only on the form of the dispersion for low energies.

4.4 Analytical Limits and Numerical Results

We now turn to the results of the calculation, detailing the analytical limits in the BCS and BEC sides as well as unitarity. To investigate the limiting form of the Green’s function, we will invert $G$ in Eq. (4.8) and simplify the notation by writing $G^{-1}(k,\omega)$ as

$$G^{-1}(k,\omega) \equiv W(k,\omega) + \frac{K^2(k,\omega)}{W^*(k,-\omega)},$$

(4.38)

defining

$$W(k,\omega) = \omega - \xi_k - \Sigma(k,\omega), \quad K(k,\omega) \equiv \Delta_0 - S(k,\omega).$$

(4.39)

When $W(k,-\omega)$ is real, we denote it by $\overline{W}(k,\omega)$.

4.4.1 Weak Coupling

We expand the Green’s function on the weak coupling side by performing an expansion in $k_F a_s$. We can immediately note that the off diagonal self energy $S \sim \Delta_0^3 \rightarrow 0$ compared to $\Delta_0$, seen by the fact that, in Eq. (4.36), $u_q v_q \sim \Delta_0$ and $\text{Im} \hat{\Gamma}_{12} \sim \Delta_0^2$ for the same reason ($L$, Eq. (4.31), has two factors of $u_p v_p$). Furthermore, the diagonal self energy becomes largely independent of $k$ and $\omega$ due to the appearance of the Hartree term. The second order term in $k_F a_s$ leads to the corresponding term in the normal Fermi liquid, Eq. (2.11), for a repulsive Galitskii gas or the attractive Fermi gas above $T_c$. We note, however, that there is still a gap in the imaginary part of the self energy which must be taken into account in evaluating the imaginary part of $M$. Denoting this term by $\delta \Sigma(k,\omega)$, we have

$$\Sigma(k,\omega) = \frac{4}{3\pi} k_F a_s \epsilon_F + \delta \Sigma(k,\omega),$$

(4.40)

where $\delta \Sigma(k,\omega) \sim (k_F a_s)^2$. Using Eq. (4.13) we then find a simple relation for $k_{\text{min}}$ correct to second order in $k_F a_s$,

$$\epsilon_{k_{\text{min}}} \simeq \mu - \Sigma_{k_{\text{min}}}(0),$$

(4.41)
where we set $\Delta = 0$ inside the self energy to polynomial orders. Using the expression for the chemical potential, which, in this limit, is exactly that for the Galitskii-Lee-Yang hard-core Fermi gas with a negative $a_s$ $[13]$, we see that the first and second order terms on the right hand side cancel, so that $k_{\text{min}} \simeq k_F$. We then find that the minimum wavevector is not determined by Hartree physics, or even by the normal state interactions. We do note, however, that the gap $\Delta$ is reduced from $\Delta_0$ by a correction which, by nonanalyticity, must be exponential in order. This is the Gorkov-Melik-Barkhudarov $[14]$ correction which arises from particle hole excitations of the medium, and is not included in the gaussian calculation. Finally, the quasiparticle weight in this limit becomes (again ignoring $S$)

$$
\frac{1}{Z^+} \simeq 1 - \frac{W}{W} \frac{\partial \Sigma}{\partial \omega} - \frac{W}{W} \frac{\partial \Sigma}{\partial \omega},
$$

and, using Eq. (4.41), we find that $W \simeq -\overline{W}$ and we can approximate $\partial_\omega \Sigma(-\omega) \simeq -\partial_\omega \Sigma(\omega)$ since we are setting $\Delta_0 \to 0$ here. The weight then becomes again the result from the hard-core Fermi gas: 1/2 with a subleading term proportional to $(k_F a_s)^2$ which decreases the weight.

### 4.4.2 Crossover Region

At unitarity ($1/k_F a = 0$), we find that there are still sharp peaks in the spectrum with large weights of $Z^+ = 0.44$ and $Z^- = 0.42$, supporting strong low-energy quasiparticles. The minimum wavevector has decreased to $k_{\text{min}} \simeq 0.83k_F$ which is larger than the mean field value of $0.77k_F$. We note a more significant difference here, however. The chemical potential is strongly renormalized with a value of $\mu = 0.40\epsilon_F$. If we compared the minimum with $k_\mu \equiv \sqrt{2m\mu}$ we would find a large difference, $k_{\text{min}} \simeq 1.3k_\mu$. In terms of the parameterization in Eq. (4.1), we compare the value of $U$ with other theories in Tbl. 4.1 and illustrate in Fig. 4.3. While the gap $\Delta$ is in good quantitative agreement with QMC results, $k_{\text{min}}$

| $|a_s| = \infty$ | $\mu/\epsilon_F$ | $U/\epsilon_F$ | $\Delta/\epsilon_F$ |
|-----------------|-----------------|----------------|-----------------|
| MFT             | 0.59            | 0              | 0.68            |
| MFT + GF        | 0.40            | -0.28          | 0.49            |
| LW $[65]$       | 0.36            | -0.50          | 0.46            |
| QMC $[76]$      | 0.42            | -0.52          | 0.50            |
| Expt $[44]$     | N/A             | -0.43          | 0.44            |

Table 4.1: Comparison of dispersion parameters with other theories. Note that the experiment value was obtained using the $\mu/\epsilon_F$ calculated from the QMC paper.
is in qualitative agreement. However, we see that the renormalization $U$ here is a quite complicated combination of $\Sigma$ and $S$ and not related to Hartree physics.

In Fig. 4.4 we compare the single particle gap $\Delta$ and quasiparticle weights $Z^+$, $Z^-$ and $Y$ with the mean field theory results. In mean field theory, the excitations at the gap have an energy equal to the order parameter for coupling values less than $1/k_F a_s \sim 0.6$ when $\mu > 0$. This is due to the fact that $\sqrt{2m\mu}$ always determines the wavevector at the bottom, and $E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta_0^2}$ is the exact energy. Furthermore, the quasiparticle weights at the minimum are all equal: $u_{k,\mu}^2 = v_{k,\mu}^2 = u_{k,\mu} v_{k,\mu} = 1/2$. Beyond the point when $\mu = 0$, $\mu$ becomes negative and $k_{\text{min}} = 0$, meaning the gap is increased, $\Delta = E_0 = \sqrt{\mu^2 + \Delta_0^2} > \Delta_0$, and the weights are now different:

$$u_0^2 = \frac{1}{2} \left( 1 + \frac{|\mu|}{\sqrt{\mu^2 + \Delta_0^2}} \right), \quad u_0^2 = 1 - u_0^2, \quad u_0^2 = \frac{\Delta_0}{2\sqrt{\mu^2 + \Delta_0^2}}. \quad (4.43)$$

In the gaussian approximation, the values for the gap, $\Delta_0$, and the weights are lowered, and follow a similar trend as in the mean field. However, the equality of $\Delta$ and $\Delta_0$ as well as the weights $Z^+$, $Z^-$ and $Y$ is split with increasing magnitude. Fluctuations increase the minimum wavevector $k_{\text{min}}$ systematically beyond the mean field solution as the coupling increases, becoming zero at a value of about 0.7, beyond the point when the chemical potential $\mu$ vanishes. This is a nontrivial result of the gaussian calculation.
4.4.3 BEC Limit

Once the wavevector $k_{\text{min}} = 0$, we see that the velocity past this point, Eq. (4.13), is trivially zero, since the derivatives of the self energy vanish due to the isotropic nature of the gas. To find the gap, we expand $\Gamma$ in small $\Delta_0/\mu$. This has been done in Ref. [77], and we find that it is only $\Sigma(0, \omega)$ that is important when $\Delta \simeq |\mu| \gg \epsilon_F$; only the collective mode contributes to the self energy and the residues can be expanded to give the Bogoliubov functions in the Bose case [77]. We then find that setting $G^{-1}(0, \Delta) \equiv 0$ gives

$$\Delta = |\mu| + \frac{\Delta_0^2}{2|\mu|} + \Sigma(0, |\mu|),$$

where $\Delta_0^2/|\mu| = 16(k_Fa_s)/3\pi$ and $\Sigma(0, |\mu|) = -2\Delta_0^2/3|\mu| < 0$ showing that $\Delta$ is decreased from the mean field result. For the quasiparticle weight, we again ignore $S$ and $\Sigma(-\Delta)$ as well as the derivatives (since they cancel at this order) to obtain

$$Z^+ = \frac{\Delta - \mu}{2\Delta - \Sigma(0, \Delta)},$$

(4.45)

Since $\mu < 0$, $|\mu| \gg \epsilon_F$, $\Delta \simeq |\mu|$ and $\Sigma(0, \Delta) \ll \epsilon_F$, we see that the quasiparticle weight actually approaches unity for positive frequencies and similarly the negative weight $Z^-$ vanishes. This can be understood physically by noting that for particle excitations, the atom-dimer interaction $a_{ad}$ scales with the atom-atom scattering length with a positive constant, such that $a_{ad} \simeq 1.2a_s$ [28], and those excitations therefore have finite weight. Hole excitations require breaking a bond in a pair which is costly in this limit.
4.5 Large-$N$ approximation

The method we use here is closely related to the $1/N$ approximation [62], and also should have the same general features as above. After including the $N$ species of fermions in the action using the hamiltonian Eq. (2.14), we perform an expansion of the partition function, or, equivalently, the Green’s function, at unitarity. One finds [62] that the self energy is of the same form as derived in the gaussian approximation, Eqs. (4.33) and (4.34), but with an overall factor of $1/N$, due to the same vertex factors discussed in Sec. 2.3. Moreover, the values for the order parameter $\Delta_0$ and $\mu$ are obtained from the mean field expression which is $0^\text{th}$ order in $1/N$. We can then derive the expressions for the dispersion minimum and gap. The gap in terms of the self energies is [62]

$$\Delta \simeq \Delta_0 + \frac{1}{2N} \left[ \Sigma(\Delta_0) - \Sigma(-\Delta_0) - 2S(\Delta_0) \right],$$

where the self energy is calculated at the mean field minimum, $k_\mu$. At unitarity its evaluation yields

$$\frac{\Delta}{\epsilon_F} \simeq 0.6864 - \frac{0.196}{N} + \mathcal{O}(N^{-2}),$$

where 0.6864 is the mean field order. Indeed, the inequality $\Delta < \Delta_0$ holds, and the threshold in the spectral function would occur at the value of $\Delta_0$. Therefore, one does obtain a sharp $\delta$-function peak in the single particle spectrum to this order. In setting the velocity to zero we obtain the correction to the mean field value for the minimum, $k_{\min} \simeq k_\mu + \delta k_{\min}/N$.

We find

$$\delta k_{\min} = \frac{1}{2} k_\mu \frac{\mu^{1/N}}{\mu^0} - \frac{1}{4m} \frac{\Sigma(\Delta_0) + \Sigma(-\Delta_0)}{\mu^0} - \frac{m\Delta_0}{4\mu^0} \left[ \partial_k \Sigma - \partial_k \Sigma - 2\partial_k S \right],$$

and by numerical evaluation we obtain $\delta k_{\min} \simeq 0.11k_F$, pushed outward from the mean field value. The quasiparticle weight in $1/N$ is

$$Z^+ \simeq \frac{1}{2} \left[ 1 + \frac{\Delta^{1/N}}{\Delta^0} + 2 \frac{\delta k_{\min}}{k_\mu} \frac{\mu^{1/N}}{\mu^0} + \frac{1}{2} \frac{\Sigma(\Delta_0) + \Sigma(-\Delta_0)}{\Delta^0} + \frac{1}{2} \left( \partial_\omega \Sigma - \partial_\omega \Sigma - 2 \partial_\omega S \right) \right],$$

and we obtain a reduced value $Z^+ \simeq (1 - 0.072/N)/2$ for this as well. We find that the $1/N$ approximation in fact also supports quasiparticles.
4.6 Conclusions

We have shown that, using general considerations of neutral fermions, coupled to gapless phonon modes, with a gapped excitation spectrum, one can derive a selfconsistent argument which supports well-defined quasiparticles in ultracold Fermi gases at zero temperature. Using the gaussian approximation throughout the BEC-BCS crossover and the large-$N$ approximation at unitarity we have illustrated the dispersion by calculating the single particle gap, quasiparticle weights, and the shift in the wavevector of the dispersion $k_{\text{min}}$, finding qualitative agreement with other theories and experiments. We find that sharp quasiparticles do exist in the system throughout the BEC-BCS crossover, even at unitarity, with strong weights. We find that $k_{\text{min}}$ is systematically shifted from the expression for the mean field value, $\sqrt{2m\mu}$, a nontrivial result.

4.7 Technical Details of the General Argument

In this appendix we make explicit the discussion in Sec. 4.2 by expanding the integrals. We first perform the integral Eq. (4.19) and (4.20) for the imaginary parts of the self energy to lowest order in $\tilde{\omega} \equiv \omega - \Delta$ for $\omega > 0$ to yield

\begin{align}
\text{Im } \Sigma(\omega) &\simeq -\alpha_\Sigma(\omega - \Delta), \\
\text{Im } \Sigma(-\omega) &\simeq -\alpha_\Sigma(\omega - \Delta), \\
\text{Im } S(\omega) &\simeq -\alpha_S(\omega - \Delta),
\end{align}

(4.50)

(4.51)

(4.52)

where we’ve defined the coefficients

\begin{align}
\alpha_\Sigma &\equiv \frac{\zeta}{4\pi} Z^-, \\
\alpha_\Sigma^+ &\equiv \frac{\zeta}{4\pi} Z^+, \\
\alpha_S &\equiv \frac{\zeta}{4\pi} Y.
\end{align}

(4.53)

The linear behavior of the imaginary parts of the self energy lead directly to the following forms for the real parts of the self energy

\begin{align}
\text{Re } \Sigma(\omega) &\simeq \Sigma_L(\omega) + \frac{\alpha_\Sigma}{\pi}(\omega - \Delta) \ln(\omega - \Delta), \\
\text{Re } \Sigma(-\omega) &\simeq \Sigma_L(\omega) - \frac{\alpha_\Sigma}{\pi}(\omega - \Delta) \ln(\omega - \Delta), \\
\text{Re } S(\omega) &\simeq S_L(\omega) + \frac{\alpha_S}{\pi}(\omega - \Delta) \ln(\omega - \Delta),
\end{align}

(4.54)

(4.55)

(4.56)

where we’ve taken out explicitly the leading logarithmic dependence, the subscript $L$ denoting that those quantities have corrections to leading order in $\tilde{\omega} \equiv \omega - \Delta$. Before we investigate the consequences for the Green’s function, we note here that this behavior has been pointed out before [78], and it was claimed that the quasiparticle weight would therefore necessarily be zero. This is due to the relation between the quasiparticle weight and
the self energy in the *normal* state

\[ Z_N = \frac{1}{1 - \frac{\partial \Sigma}{\partial \omega}|_{\omega=0}}, \quad (4.57) \]

which, with the behavior in the *superfluid* state, would be zero when evaluated at \( \omega = \Delta \). We point out that it is Eqs. (4.11) and (4.12) which determine the weights, and we will show that this is finite in the current expansion. By expanding the real and imaginary parts of \( G^{-1} \) in Eq. (4.38) we obtain

\[ \text{Im } G^{-1}(\omega) = -\frac{\tilde{\omega}}{W(\Delta)} \left[ J_1 + J_2 + 2J_1 \left( \frac{\partial \omega K_L}{K(\Delta)} - \frac{\partial \omega W_L}{W(\Delta)} \right) \tilde{\omega} - \frac{2}{\pi} \left( \frac{J_1}{K(\Delta)} \right)^2 \tilde{\omega} \ln \tilde{\omega} + O(\tilde{\omega}^2 \ln \tilde{\omega}) \right] \quad (4.58) \]

and

\[ \text{Re } G^{-1}(\omega) = \frac{1}{W(\Delta)} \left[ R\tilde{\omega} + \frac{J_1 + J_2}{\pi} \tilde{\omega} \ln \tilde{\omega} + O(\tilde{\omega}^2 \ln \tilde{\omega}) \right], \quad (4.59) \]

where we’ve defined the shorthand

\[ J_1 \equiv \alpha \Sigma W(\Delta) - \alpha_S K(\Delta), \quad J_2 \equiv -\alpha \Sigma W(\Delta) - \alpha_S K(\Delta), \quad (4.60) \]

and the derivatives are evaluated at \( \Delta \), \( \overline{W}(\omega) \equiv W(-\omega) \), and the subscript \( L \) indicates we differentiate the corresponding part of the self energies. The number \( R \) is

\[ R \equiv W \partial_\omega \overline{W} + 2 K \partial_\omega K_L + \overline{W} \partial_\omega W_L \quad (4.61) \]

We now make the crucial observation that \( J_1 = J_2 = 0 \), using the general relations Eqs. (4.12). We can therefore verify that the spectral function vanishes as \( \tilde{\omega} \to 0 \) at most like \( \tilde{\omega} \ln \tilde{\omega} \). We note that the prefactor (and the next leading order corrections) will depend on secondary corrections to the approximations made in this appendix to the effective interaction, the Green’s function itself, and the additional diagrams we have neglected, all of which are complicated but not required for the current argument. The quasiparticle weight is given by

\[ Z^+ = \frac{R(\Delta)}{W_L(-\Delta)} \quad (4.62) \]

and is related to \( Z^- \) and \( Y \) again by Eqs. (4.12). We now have no more information about these quantities in general, except to say there’s no reason to believe they vanish unless one encounters a quantum phase transition.
Chapter 5

Bogoliubov-deGennes Analysis of Inhomogeneous Atomic Gases

An important aspect of cold atom experiments is the presence of a harmonic trap, which we have ignored in this thesis until now. A "local density" or Thomas-Fermi Approximation (TFA) [9] has usually been adequate to take this into account. The TFA asserts that the properties at point \( r \) in a 'slowly varying' potential \( V_{\text{trap}}(r) \) are the same as those of the uniform gas at a chemical potential \( \mu_\sigma(r) = \mu_\sigma - V_{\text{trap}}(r) \) with \( \sigma = \uparrow, \downarrow \). This leads to the simple result that the spatial dependence of any observable must follow contours of constant trapping potential, which is directly testable for the densities \( n_\sigma(r) \). Two experiments on polarized, unitary Fermi gases find rather different results with respect to the TFA. The MIT group [24, 26, 27], with a large number of atoms \( N = 10^7 \) and a small trap anisotropy \( 1/\alpha = \omega_r/\omega_z \simeq 5 \), finds that the densities follow contours of \( V_{\text{trap}}(r) \). On the other hand, the Rice group [81], with smaller \( N = 10^5 \) and larger anisotropy \( 1/\alpha \simeq 50 \) observes gross violations of the equipotential contour condition for the densities [82].

Motivated by this, we have investigated the validity of the TFA using the zero temperature BdG equations [87, 88] and derived scaling arguments for the unitary gas in anisotropic, three dimensional traps with polarization up to 40\%. Our main results are:

- The numerical calculation exhibits order parameter oscillations which might be interpreted as the signature of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase, however, they must be interpreted with care. We find that, in the symmetric trap, the oscillations are a numerical artifact and disappear as the calculation is done more accurately.
- We find that the size of the region between the unpolarized superfluid and the polarized normal states can be described as an interface between the two in the symmetric trap.

\footnote{This work was done in collaboration with R. Sensarma, R. Dienzer and M. Randeria. Ref. [83] contains our preliminary work, which are superseded by the results described in this chapter. For other recent theoretical developments, see Parish and Huse [84] and Baksmaty et al. [85]. The most recent experiments of the Rice group [86] seem to give evidence for the non-equilibrium effects proposed in [84]. Nevertheless, we describe here our own work which focuses on equilibrium physics in anisotropic traps.}
trap, and does not survive in a thermodynamic limit.

• The violation of the equipotential contour criterion for the magnetization $m(r) = n_\uparrow(r) - n_\downarrow(r)$ increases with increasing anisotropy $1/\alpha$, but decreases with increasing total number of particles $N = N_\uparrow + N_\downarrow$.

• We derive a simple condition for the consistency of the TFA: $h/\omega_r = (N\alpha)^{1/3}f(P) \gg 1$, where $f$ is a function of the polarization $P = (N_\uparrow - N_\downarrow)/N$ and $h = (\mu_\uparrow - \mu_\downarrow)/2$ is half the difference in the chemical potentials. We use this $(N\alpha)^{1/3}$ scaling of $h/\omega_r$ to get a better understanding of the $N$ and $\alpha$ dependences of our BdG results.

• At a qualitative level, we are able to account for the differences between the MIT and Rice experiments with respect to the question of when the magnetization should or should not follow contours of constant potential at $T = 0$.

5.1 Bogoliubov deGennes Equations

Our approach to the problem of strongly interacting, polarized Fermi gases in anisotropic traps is to solve the BdG equations [89]. This is the simplest approach which goes beyond the TFA and is a generalization of the BCS-Leggett mean field theory for a spatially inhomogeneous gas. This method has been applied to the study of vortices in the strongly interacting regime [90], as well as the study of polarized gases in isotropic traps [87, 88]. For a single-channel description valid for the experimentally-relevant wide resonance, the Hamiltonian density for the polarized gas is (1.14) where we now add the trapping potential

$$V_{\text{trap}}(r) = \frac{1}{2}m \omega_0^2 \left( r^2 + \alpha^2 z^2 \right)$$

(5.1)

and we use cylindrical coordinates $r = (r, \theta, z)$. The asymmetry of the trap is defined as $\alpha^{-1}$ so that larger asymmetry in the $z$-direction corresponds to larger values of $\alpha^{-1}$. We define the average chemical potential and the difference as

$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}, \quad h = \frac{\mu_\uparrow - \mu_\downarrow}{2},$$

(5.2)

respectively. The mean field state is found through the solution of the BdG equations (which are derived in Sec. 5.4)

$$\begin{pmatrix} H_0(r) - \mu & \Delta(r) \\ \Delta^*(r) & -H_0(r) + \mu \end{pmatrix} \begin{pmatrix} u_i(r) \\ v_i(r) \end{pmatrix} = E_i \begin{pmatrix} u_i(r) \\ v_i(r) \end{pmatrix},$$

(5.3)

where $H_0(r) = -\nabla^2/2m + V(r)$, together with the gap equation

$$\Delta(r) = g(k_c) \sum_{E_i > h} u_i(r)v_i^*(r),$$

(5.4)
polarization

\[ m(r) = \sum_{0 \leq E_i < h} (|u_i(r)|^2 + |v_i(r)|^2), \quad (5.5) \]

and density

\[ n(r) = m(r) + \sum_{E_i > h} 2|v_i(r)|^2, \quad (5.6) \]

at zero temperature. We use the notation \( k_c \) to denote the cutoff energy due to the contact interaction, preferring to use \( \Lambda \) for a different definition (see Eq. (5.13)) later on in this chapter. These equations are solved self-consistently for \( \Delta(r) \), \( \mu \) and \( h \) using the constraints that the total number of particles \( N \) and polarization \( P \) are

\[ N = \int d^3r n(r), \quad P = N^{-1} \int d^3r m(r). \quad (5.7) \]

The solution of these equations is simplified if we expand the wavefunctions \( u_i \), \( v_i \) in terms of the eigenfunctions of the diagonal piece \( H_0(r) - \mu \). Measuring lengths in units of the radial harmonic oscillator length \( a_0 = \sqrt{\hbar/m\omega_0} \) and energies in units of \( \omega_0 \), these functions are

\[ \phi_{np\ell} = f_{p\ell}(r) \exp(i\ell\theta)g_n(z)/\sqrt{2\pi}, \quad (5.8) \]

where the radial and axial functions are related to associated Laguerre and Hermite polynomials,

\[ f_{p\ell}(r) = \sqrt{p!/(p+\ell)!}e^{-r^2/2}r^\ell L_p^\ell(r^2), \quad (5.9) \]
\[ g_n(z) = \sqrt{\sqrt{\alpha}/(2^n\sqrt{\pi}n!)}e^{-\alpha z^2/2}H_n(\sqrt{\alpha}z), \quad (5.10) \]

respectively. The corresponding eigenvalue is \( \epsilon_{np\ell} = (2p+\ell+1) + \alpha(n+1/2) - \mu \). The BdG Hamiltonian is block-diagonal in \( \ell \) due to azimuthal symmetry, so for a given \( \ell \) we need to diagonalize

\[ H^{(\ell)} = \begin{pmatrix} T^{(\ell)} & \Delta^{(\ell)} \\ \Delta^{(\ell)} & -T^{(\ell)} \end{pmatrix}, \quad (5.11) \]

where \( T^{(\ell)}_{nn'pp'} = \epsilon_{n\ell p}\delta_{nn'}\delta_{pp'} \) and \( \Delta^{(\ell)}_{nn'pp'} = \int_0^\infty rdr \int_{-\infty}^\infty dz f_{p\ell}(r)f_{p'\ell}(r)g_n(z)g_{n'}(z)\Delta(r,z) \)

Since \( \Delta(r,z) = \Delta(r,-z) \), the only non-zero matrix elements of \( \Delta^{(\ell)}_{nn'pp'} \) correspond to even \( n + n' \).

Normally, the bare coupling \( g(k_c) \) in Eqs. (5.3), (5.4) is replaced with the scattering length using Eq. (1.13), however, here we numerically introduce an energy cutoff on \( \epsilon_{np\ell} \) to
Figure 5.1: The chemical potentials $\mu$ (upper blue curve) and $h$ (lower red curve) for $P = 0.30$ and $N_\uparrow = 700$ in the symmetric trap ($\alpha = 1$) for a range of cutoff values $\Lambda = 6-20$. The dashed lines indicate the fit to the form $a\Lambda^{-1/2} + b$, where $b$ is the extrapolated value.

limit the number of the basis functions used, with a maximum energy of $E_c$. We therefore choose the basis cutoff

$$E_c \equiv \hbar^2 k_c^2 / 2m$$

(5.12)
to coincide with the cutoff for the regularization. In doing so, we must study the self consistent solutions as $E_c$ increases. Furthermore, in order to have a consistent set of comparisons differing by the number of particles, we choose $E_c$ to be a multiple of the Fermi energy $\epsilon_F$, so

$$E_c \equiv \Lambda \epsilon_F,$$

(5.13)

where $\epsilon_F = (6N\alpha)^{1/3}\omega_0$. To study the solutions as a function of $\Lambda$, we use an extrapolation procedure for the chemical potentials and subsequent analyses of the density profiles. The scaling of the BdG solutions can be seen by noting that the bare coupling $g(k_c) \sim 1/\sqrt{E_c}$ in Eq. (5.4), and, in order to obtain a finite result, the sum in Eq. (5.4) must increase to compensate. All quantities therefore behave as $\Lambda^{-1/2}$ tending to a constant. For illustration purposes, we plot the chemical potentials $\mu$ and $h$ against the cutoff $\Lambda$ for $N_\uparrow = 700$ and $P = 0.30$. We note that this is analogous to performing the calculation on a lattice and taking the wavevector cutoff (the natural choice of the Bravais lattice vector in the first Brillouin zone) very large to obtain the continuous limit.
Figure 5.2: (A) Majority (black) and minority (gray) density profiles and (B) order parameter $\Delta$ (black) and magnetization (grey) profiles along the axis of the trap. The solid lines are BdG results and the dashed lines are TFA results. The calculations are for a trap with $\alpha = 1/4$ containing $N = 865$ particles and a polarization of 30%.

5.2 Numerical Results

We now discuss the self-consistent solution of the BdG equations as a function of total $N = N_\uparrow + N_\downarrow$, polarization $P = (N_\uparrow - N_\downarrow) / N$ and trap anisotropy $1/\alpha$ at unitarity ($a_s = \infty$). We have extensively studied the problem for $N$ up to 2500 particles, $0 \leq P \leq 0.4$ and $\alpha = 1, 1/2, 1/4$. In Fig. 5.2(A) we plot the majority ($n_\uparrow$) and minority ($n_\downarrow$) densities along the $z$ axis for a representative data set ($\alpha = 1/4$, $N = 865$ and polarization $P = 30\%$). In Fig. 5.2(B) we plot the corresponding magnetization $m(r) = n_\uparrow(r) - n_\downarrow(r)$ together with the local order parameter $\Delta(r)$. In both panels the solid lines are BdG results, while dashed lines are TFA predictions (using the bulk phase diagram [91–93] as input).

Both the BdG and TFA results show an unpolarized superfluid at the center of the trap and a fully polarized normal gas at the edge. There is a marked decrease in the BdG central density relative to TFA, with a redistribution of minority atoms to an intermediate region. The main difference between BdG and TFA is precisely in this intermediate region. Within the TFA there is a discontinuous jump in the order parameter which is smoothed out in the BdG solution since this lowers the gradient energy. Furthermore, the order parameter exhibits oscillations that might be interpreted as evidence for a FFLO phase [94], but as we will discuss in detail below, these oscillations are, in fact, numerical artifacts and not indicative of a FFLO region.
5.2.1 Density Profiles

We begin our test of the TFA by increasing the trap anisotropy $1/\alpha$. In the top panel of Fig. 5.3 we plot the magnetization $m(r,z)$ for $N = 865$ particles with $P = 30\%$ polarization and $\alpha = 1, 1/2, 1/4$. In the lower panel we show the corresponding plots of the column-integrated magnetization, which is simpler to measure in experiments, and is given by $m_{col}(y,z) = \int_{-\infty}^{\infty} dx m(\sqrt{x^2 + y^2}, z)$. For the spherical case ($\alpha = 1$) the equipotential contour condition must be satisfied by symmetry. As the anisotropy $\alpha^{-1}$ increases we see that the magnetization gets more concentrated along the wings. Moreover, the boundary between the magnetized and unmagnetized regions near the $z = 0$ plane becomes straighter, yielding a magnetization “hole” that becomes more rectangular. This is very similar to the observed profiles in the Rice experiments [81].

To understand why the MIT results look so different, we must study the dependence on the total number of particles, for a fixed trap anisotropy and polarization. In Fig. 5.4 we plot the results for (from top to bottom) $N = 865$, 1538, and 2307 particles in a trap with $\alpha = 1/2$ and $P = 30\%$. For the smallest $N$ the magnetization is localized along the axis, and is seen to spread out toward the radial direction with increasing $N$. The largest $N$ results show a rather elliptical magnetization density indicating that the magnetization begins to follow the equipotential contours as $N$ increases.

5.2.2 Interface region

The existence of a magnetized superfluid region implies the breakdown of the TFA, since there is no such phase for a uniform gas in the thermodynamic limit at unitarity and this region could be stabilized only by the presence of a trap. Earlier BdG studies in
isotropic traps [87, 88] have found such a FFLO-like region but, as we discuss next, one must be very careful to interpret numerical results to address this question. To illustrate the absence of these oscillations we first restrict ourselves to the symmetric trap where $\alpha = 1$ in which the cutoff $\Lambda$ can be increased to a large value. Fig. 5.5 shows a clear trend of the decreasing oscillation amplitude, and indeed it is completely quenched by a value of $\Lambda = 30$. This decreasing trend is found for every particle number $N$ studied, however, as $N$ increases one must increase the cutoff to higher values to see the oscillation completely quenched, due to the steepness of the slope of $\Delta$ approaching this region. We therefore attribute the oscillations to a numerical artifact arising from the finite cutoff analogous to the Gibbs phenomena in Fourier series. For anisotropic traps, even though we have seen the amplitude decrease in our data, we do not have the extensive cutoff calculation as at $\alpha = 1$. The calculation time for anisotropic traps scales with the cutoff $\Lambda$, asymmetry $\alpha^{-1}$ and majority particle number $N_\uparrow$ as $\Lambda^6N_\uparrow^2\alpha^{-1}$, which can be shown by considering the cube of the dimension of the largest $\ell$ matrix which is determined by the quantum numbers of $E_c$.

Since we have ruled out FFLO behavior in the intermediate region, it is important to ask whether the region can be described as an interface with a surface energy [82]. To investigate this, let us now study the fraction of the majority species $n_{\text{int}}$ in this region as a function of $N_\uparrow$, as well as its size $\Delta R_{\text{int}}$, defined by the existence of both the local
polarization \( p(r) = m(r)/n(r) \) and density of minority particles \( n_↓(r)/n(r) \) scaled by the local total density. The fraction of majority particles, then, is defined by

\[
  n_{\text{int}} = N↑^{-1} \int_{\Delta R_{\text{int}}} d^3r \, n↑(r). \tag{5.14}
\]

For simplicity, we again work in a symmetric trap. We can make a simple argument to explain the behavior of \( n_{\text{int}} \) and \( \Delta R_{\text{int}} \) with \( N↑ \) by modeling the region as a shell and using the Thomas-Fermi scaling for the radius of the cloud \( R_{TF} \). The radius scales as the Fermi energy like

\[
  R_{TF,↑} = \sqrt{\frac{2\epsilon_F}{ma^2}} = \sqrt{2}(6N↑)^{1/6}a_0, \tag{5.15}
\]

where we have used the definition of the Fermi energy and the oscillator length \( a_0 \). The average density in the cloud is \( \bar{n} \sim N↑/R_{TF,↑}^3 \). Multiplying by the shell volume, \( \Delta R_{\text{int}}R_{TF,↑}^2 \) we obtain the number of particles in the shell. Dividing by the total number of majority particles we obtain

\[
  n_{\text{int}} \sim \frac{\bar{n} \Delta R_{\text{int}} R_{TF,↑}^2}{N↑} \sim \frac{\Delta R_{\text{int}}}{R_{TF,↑}}. \tag{5.16}
\]

For an interface description, \( \Delta R_{\text{int}} \sim k_F^{-1} \sim N↑^{-1/6} \) and therefore \( n_{\text{int}} \sim N↑^{-1/3} \). We find in Fig. 5.6 that, indeed, \( n_{\text{int}} \) and \( \Delta R_{\text{int}} \) scale with \( N↑ \) and tend to vanish as \( N↑ \) increases. We also note that if one were not to use the extrapolation procedure we use here, one
Figure 5.6: Left: Fraction of majority particles $n_{\text{int}}$, defined in Eq. (5.16) in the intermediate region as a function of $N_\uparrow$ in a symmetric trap ($\alpha = 1$) and $P = 30\%$. The top curve uses a cutoff of $\Lambda = 8$ and tends to a finite value, while the lower curve is extrapolated to $\Lambda \to \infty$, and tends to zero. Right: Size of the intermediate region, extrapolated to $\Lambda \to \infty$, for the same parameters. In both graphs, $N$ ranges from 462 to 1077.

would incorrectly conclude that the intermediate region exists in the thermodynamic limit, tending to a value of $n_{\text{int}} \simeq 0.20$.

5.2.3 Scaling with $N$ and $\alpha$

We now derive a criterion for the consistency of the TFA and compare our results for the chemical potentials plotted in Fig. 5.7. We start with the Thomas-Fermi theory (dashed lines in Fig. 5.2) using the densities from the bulk phase diagram [91–93]

\[
\begin{align*}
n_\uparrow[\mu(x)] &= \begin{cases} 
\frac{1}{6\pi^2} \left[ \frac{2m\mu(x)}{\beta} \right]^{3/2} & \mu(x) > 1.28h_0 \\
\frac{1}{6\pi^2} \{2m[\mu(x) + h_0]\}^{3/2} & 1.28h_0 > \mu(x) > -h_0 \\
0 & -h_0 > \mu(x)
\end{cases} \\
n_\downarrow[\mu(x)] &= \begin{cases} 
\frac{1}{6\pi^2} \left[ \frac{2m\mu(x)}{\beta} \right]^{3/2} & \mu(x) > 1.28h_0 \\
\frac{1}{6\pi^2} \{2m[\mu(x) - h_0]\}^{3/2} & 1.28h_0 > \mu(x) > h_0 \\
0 & h_0 > \mu(x)
\end{cases}
\end{align*}
\]

(5.17) (5.18)

where $\mu_\sigma = \mu_{\sigma,0} - V(x)$, so that $\mu(x) = (\mu_\uparrow(x) + \mu_\downarrow(x))/2 \equiv \mu_0 - V(x)$ and $h = (\mu_\uparrow(x) - \mu_\downarrow(x))/2 \equiv h_0$ is independent of $x$. Our goal is to integrate these expressions to obtain the numbers of particles in each region. After scaling the resulting integrals we
obtain

\[ N_{\sigma}^{SF} = \frac{16}{3\pi \alpha} \left( \frac{h_0}{\omega_0} \right)^3 I_1 \left( \frac{\mu_0}{h_0} \right) \]  \hspace{1cm} (5.19) \\
\[ N_i^N = \frac{16}{3\pi \alpha} \left( \frac{h_0}{\omega_0} \right)^3 I_2 \left( \frac{\mu_0}{h_0} \right) \]  \hspace{1cm} (5.20) \\
\[ N_i^\downarrow = \frac{16}{3\pi \alpha} \left( \frac{h_0}{\omega_0} \right)^3 I_3 \left( \frac{\mu_0}{h_0} \right) \]  \hspace{1cm} (5.21)

where \( I_n \) are integrals that only depend on the ratio \( \mu_0/h_0 \) of the chemical potential sum and difference. We can then write down the expression for the polarization as a function of \( \mu_0/h_0 \), and in principle can be inverted to obtain the ratio as a function of \( P \). Finally, we obtain \( h_0/\omega_0 = (N\alpha)^{1/3} f(P) \), where \( f(P) \) is a numerically determined monotonically increasing function of \( P \) which goes like \( P^{2/5} \) for \( P \ll 1 \) and is of order unity for the \( P \) values of interest here. We note that a similar criterion (without an explicit \( P \)-dependence) for the violation of the equipotential-contour condition was derived in Ref. [82] using a different approach.

We have checked that the \( \text{BdG} \) results for \( h_0/\omega_0 \) are consistent with \( (N\alpha)^{1/3} \) scaling even though the values are smaller than the \( \text{TFA} \) estimates. If the condition \( h_0/\omega_0 \gg 1 \) is violated the \( \text{TFA} \) will breakdown, and how this breakdown manifests itself in various quantities turns out to be strongly dependent on the anisotropy \( 1/\alpha \) both in the \( \text{BdG} \) results and in the experiments. For the symmetric trap we have good agreement for \( h \) in the entire range of \( N \) studied, as shown in Fig. 5.7. The violation of the equipotential contour criterion is also absent, as seen in Fig. 5.4, however, it grows progressively with \( 1/\alpha \) as seen from our \( \text{BdG} \) results. The size of the intermediate region also grows with \( 1/\alpha \) as discussed above. We then understand why the MIT experiments, with \( (N\alpha)^{1/3} \approx 100 \) and a small anisotropy, show that the equipotential contour criterion is obeyed, while the Rice experiments \( (N\alpha)^{1/3} \approx 10 \) and a large anisotropy shows significant violation of this criterion.

### 5.3 Conclusions

In this chapter we have shown that one must be careful to interpret the occurrence of oscillations of the order parameter in numerical \( \text{BdG} \) calculations due to a finite cutoff in the calculation, and provided a method of studying as a function of the cutoff. Furthermore, we have shown that the intermediate region behaves like an interface for an isotropic trap, and that its shape does not follow contours of constant trap potential as the asymmetry increases. Finally, we have derived a consistency criterion for the agreement of the calculation with the \( \text{LDA} \) and shown it to have good agreement with the difference between the chemical potentials in the isotropic trap. Further study would include all the above questions for
Figure 5.7: The chemical potentials $\mu$ (blue) and $h$ (red) for $P = 0.30$ in the symmetric trap ($\alpha = 1$) for a range of numbers of particles with $N = 1400 - 15000$. The brown dotted line indicates the Thomas-Fermi prediction for $h$.

stronger polarization and asymmetry, however, due to the high scaling of the calculation with the basis cutoff and asymmetry, studying the equipotential contour criterion and cutoff scaling would be very expensive.

5.4 Derivation of BdG Equations

Here we develop the BdG equations from the action of Eq. (4.27). We return to the effective action of the bosonic field $\Delta(x, \tau)$

$$S_{\text{eff}}[\Delta^*, \Delta] = \int d^4x \frac{|\Delta(x)|^2}{g_\Lambda} - \text{Tr} \ln \hat{G}^{-1},$$

(5.22)

where the Trace is over both Nambu and basis function indices (either coordinate or momentum space) Consider now a static, but spatially varying, saddle point approximation for the field $\Delta(r, \tau) = \Delta(r)$. The saddle point equation is again given by $\delta S_{\text{eff}}/\delta \Delta^*(r) = 0$, or

$$\frac{\Delta(r)}{g_\Lambda} = - \int d^4x \text{ tr} \hat{G}(x, \tau) \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

(5.23)
The goal here is to change the trace from the Nambu index to that which diagonalizes \( \hat{G} \). To do that, consider \( \hat{G}^{-1}(r, i\omega_n) \) in Matsubara frequency. We have

\[
\hat{G}^{-1}(r, i\omega_n) = \begin{pmatrix}
  i\omega_n - H_0(r) + (\mu + h) & \Delta(r) \\
  \Delta^*(r) & i\omega_n + H_0(r) - (\mu - h)
\end{pmatrix}
\]

(5.24)

and define a (time independent) basis transformation \( U(r) \) which diagonalizes \( \hat{G}^{-1}(r, i\omega_n) \),

\[
\hat{U}_n = \begin{pmatrix}
  u_n(r) & -v_n^*(r) \\
  v_n(r) & u_n^*(r)
\end{pmatrix},
\]

(5.25)

where the two columns give the eigenvalues \( E_n + h \) and \( -E_n - h \), respectively.

Now \( \hat{G}^{-1}(r, i\omega_n) = (i\omega_n + h)\hat{\sigma}_0 + \hat{H}_{\text{bdg}}(r) \) where \( \hat{H}_{\text{bdg}} \) is the BdG matrix for equal population with chemical potential \( \mu \), and is the matrix in Eq. (5.3). We define its eigenfunctions and eigenvalues by \( \phi_n = [u_n(r), v_n(r)] \) and \( E_n \). Due to particle-hole symmetry there are also eigenfunctions \( \phi_{-n} = [-v_n^*(r), u_n^*(r)] \) with energy \( -E_n \). It is evident that \( \phi_n \) and \( \phi_{-n} \) are the eigenfunctions of \( \hat{G}^{-1}(r) \) with eigenvalues \( E_n \uparrow = E_n - h \) and \( -E_n \downarrow = -E_n - h \), respectively. We then write

\[
\hat{U}_n \hat{G}^{-1} \hat{U}_n^\dagger = \begin{pmatrix}
  i\omega_n - E_n \uparrow & 0 \\
  0 & i\omega_n + E_n \downarrow
\end{pmatrix}
\]

(5.26)

and invert the equation to insert into the saddle point equation. We obtain

\[
\frac{\Delta(x)}{g\Lambda} = \sum_{mn} \text{tr} \left( (i\omega_m - E_n \downarrow)^{-1} \begin{pmatrix}
  0 & 0 \\
  0 & (i\omega_m + E_n \uparrow)^{-1}
\end{pmatrix} \right) \hat{U}_n^\dagger a \hat{U}_n,
\]

(5.27)

where

\[
\hat{U}_n^\dagger a \hat{U}_n = \begin{pmatrix}
  v_n^*(x)u_n(x) & -|v_n(x)|^2 \\
  |u_n(x)|^2 & -v_n^*(x)u_n(x)
\end{pmatrix}
\]

(5.28)

and, on doing the Nambu Trace and the Matsubara sums, the saddle point equation reduces to

\[
\Delta(x) = g\Lambda \sum_n [1 - f(E_n \downarrow) - f(E_n \uparrow)] u_n(x)v_n^*(x),
\]

(5.29)

where \( f(z) \) is the Fermi function. Note that it reduces to Eq. (5.4) in the limit of zero temperature.

The number densities of the two species fixes the two chemical potentials through the
equations $n_\sigma = - \partial \Omega / \partial \mu_\sigma$ with $\Omega = S_{\text{eff}} / \beta$. These reduce to the following equations

\[ n_\uparrow = \text{Tr} \hat{G} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad n_\downarrow = - \text{Tr} \hat{G} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \] (5.30)

Now, using the same transformation above and computing

\[ \hat{U}_n^\dagger \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \hat{U}_n = \begin{pmatrix} |u_n(x)|^2 & -u_n^*(x)v_n(x) \\ -u_n(x)v_n(x) & |v_n(x)|^2 \end{pmatrix} \] (5.31)

and

\[ \hat{U}_n^\dagger \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \hat{U}_n = \begin{pmatrix} |v_n(x)|^2 & u_n^*(x)v_n(x) \\ u_n(x)v_n(x) & |u_n(x)|^2 \end{pmatrix}, \] (5.32)

we get the following equations after the Matsubara sums

\[ n_\uparrow = \int d^3r \sum_n |v_n(r)|^2 [1 - f(E_{n\uparrow})] + f(E_{n\uparrow})|u_n(r)|^2 \] (5.33)

and

\[ n_\downarrow = \int d^3r \sum_n |v_n(r)|^2 [1 - f(E_{n\downarrow})] + f(E_{n\downarrow})|u_n(r)|^2, \] (5.34)

where, in obtaining the last equation one has to take $\omega_n \Rightarrow -\omega_n$ before before doing the Matsubara sums. By constructing the total density $n = n_\uparrow + n_\downarrow$ and magnetization $m = n_\uparrow - n_\downarrow$ and taking the zero temperature limit, we obtain Eqs. (5.5) and (5.6).
Chapter 6

Hydrodynamic Analysis of Colliding Atomic Gases

Advances in the ability to manipulate dilute, ultra-cold gases have opened up new frontiers in the study of non-equilibrium dynamics of strongly interacting quantum systems. In contrast to electronic systems, the Fermi energy in typical trapped alkali atom gas experiments is of the order of a few kHz, meaning that dynamics can be observed in real time, on the order of milliseconds and questions about metastability and equilibration in quantum systems can now be explored in the laboratory.

A striking example of such non-equilibrium dynamics was reported recently by Sommer et al. [6], who studied the collision of two clouds of ultra-cold fermions prepared in different spin states. In the strongly interacting regime, they observed the remarkable phenomenon of the two clouds bouncing off each other for several periods, before the motion is damped out leaving the two clouds sitting side-by-side on intermediate time scales. At long times, the two clouds slowly merge together, and the long-time dynamics was analyzed in detail in Ref. [6] in terms of spin diffusion.

We focus here\textsuperscript{5} on the remarkable behavior at short and intermediate time scales. Here we address:

- The reason that the strongly interacting clouds bounce off each other and then settle down next to each other for time scales up to several hundred milliseconds.
- Concentrating on the strongly interacting regime near unitarity, where the $s$-wave scattering length $a_s$ is infinite, we comment on how the dynamics changes with decreasing $k_F a_s > 0$.

\textsuperscript{5}This work was done in collaboration with E. Taylor, S. Zhang, and M. Randeria [95]. The author was mostly responsible for some preparatory numerical work which was not part of the publication, and also helped with the numerical work in solving the lowest order constraint variational (LOCV) and hydrodynamic equations.
Figure 6.1: Schematic picture of the experiment of Sommer et al. [6]. Two spin-polarized clouds are separated on top of harmonic trap.

6.1 Theoretical Treatment

6.1.1 Hydrodynamics

We consider here the collision of two spin-polarized clouds, each made up entirely of atoms with different spin, \( \sigma = \uparrow \) or \( \downarrow \), that are initially separated spatially in the \( z \)-direction, illustrated in Fig. 6.1. Our main hypothesis is that the collisions between atoms in the two clouds are sufficiently rapid to establish local thermodynamic equilibrium when the clouds overlap. Thus the clouds behave hydrodynamically in the overlap region and their dynamics reflect the equation of state of the gas. At unitarity, the two-body collision rate \( 1/\tau_2 \sim \epsilon_F \) [96, 97], where we set \( \hbar = k_B = 1 \), for a range of temperatures \( 0.1 < T/\epsilon_F < 0.3 \). With a Fermi energy \( \epsilon_F \sim 10^4 \text{Hz} \) and an axial trap frequency \( \omega_z \sim 10 \text{Hz} \) [6], the gas in the overlap region of the clouds will reach local thermodynamic equilibrium within \( \sim 10^{-3} \) trap periods of the start of the collision. We note that hydrodynamics also describes well the very different behavior observed in colliding clouds of \textit{spin-balanced} gases [98] at unitarity.

The spin \( \uparrow \) and \( \downarrow \) atoms are initially in scattering states, and the formation of two-body bound states requires three-body collisions in order to satisfy kinematic constraints. The time scale \( \tau_3 \) for such processes close to unitarity has not been studied extensively, however, there are indications that \( 1/\tau_3 \) is suppressed close to unitarity [99]. In addition, the \( \tau_3 \) relevant to the experiment of Ref. [6] is further enhanced relative to the microscopic three-body collision time, since such processes are limited here to a small overlap region for a fraction of the oscillation period \( \omega_z^{-1} \). All of our analysis below is valid for times \( t \ll \tau_3 \).

Thus for the time scales \( \tau_2 \ll t \ll \tau_3 \), we model the collisional dynamics of the two spin-polarized clouds using Euler’s equation

\[
\frac{\partial v_\sigma}{\partial t} + \nabla v_\sigma^2 = -\nabla \left( \frac{\partial E}{\partial n_\sigma} + V_{\text{trap}} \right) - \gamma v_\sigma
\]  

(6.1)
and the continuity equation
\[ \frac{\partial n_\sigma}{\partial t} + \nabla \cdot (n_\sigma v_\sigma) = 0. \]  
(6.2)

Here \( v_\sigma \) and \( n_\sigma \) are the velocity and density of the \( \sigma \) fermions, \( V_{\text{trap}} = m(\omega_\perp^2 \rho^2 + \omega_z^2 z^2)/2 \) is the trap potential. The energy density functional \( \mathcal{E}[n_\sigma(r)] \) will be discussed in detail below. We include a phenomenological \( \gamma \) to account for strong spin-current damping in the hydrodynamic regime \cite{100,101}. Viscous damping, which describes the damping of in-phase current \( (\mathbf{v}_\uparrow = \mathbf{v}_\downarrow) \), is ignored since the viscosity is small at unitarity \cite{96,97,102}, and the motion of the colliding clouds is primarily out-of-phase.

The most relevant dynamical variables to the problem of two colliding clouds are the centers-of-mass of the two clouds and their widths. Using the notation
\[ \langle \cdots \rangle_\sigma \equiv 1/N_\sigma \int d^3r n_\sigma(\cdots), \]  
(6.3)
we define the the center-of-mass position of the \( \sigma \) component as \( \bar{z}_\sigma \equiv \langle z \rangle_\sigma \) and its width as \( \delta z_\sigma \equiv \sqrt{8 \langle (z - \bar{z}_\sigma)^2 \rangle_\sigma} \) so that \( \delta z_\sigma \) coincides with the axial \textit{Thomas-Fermi} (TF) radius \( R_\alpha \) in equilibrium. The hydrodynamic equations (6.1) and (6.2) then lead to the exact equations of motion:
\[ \ddot{\bar{z}}_\sigma + \omega_z^2 \bar{z}_\sigma = \frac{-1}{m} \left\langle \partial_z (\partial \mathcal{E}/\partial n_\sigma) \right\rangle_\sigma - \langle \gamma v_{\sigma z} \rangle_\sigma + \langle v_\sigma \cdot \nabla v_{\sigma z} - \partial_z v_\sigma^2/2 \rangle_\sigma \]  
(6.4)
and
\[ \ddot{\delta z}_\sigma + \omega_z^2 \delta z_\sigma = 8 \frac{\langle v_{\sigma z}^2 \rangle_\sigma}{\delta z_\sigma} - \frac{\langle \delta z_\sigma^2 \rangle_\sigma}{\delta z_\sigma} - 8 \frac{\langle \dot{\delta z}_\sigma \rangle_\sigma^2}{\delta z_\sigma} - \frac{8}{m \delta z_\sigma} \langle (z - \bar{z}_\sigma) \partial_z (\partial \mathcal{E}/\partial n_\sigma) \rangle_\sigma - \frac{8}{\delta z_\sigma} \langle (z - \bar{z}_\sigma) \gamma v_{\sigma z} \rangle_\sigma \]  
(6.5)
\[ + \frac{8}{\delta z_\sigma} \langle (z - \bar{z}_\sigma) [v_\sigma \cdot \nabla v_{\sigma z} - \partial_z v_\sigma^2/2] \rangle_\sigma. \]

We solve these equations using a TF ansatz
\[ n_\sigma(r,t) = \frac{\alpha(2m\epsilon_F^0)^{3/2}}{6\pi^2 \delta z_\sigma(t)} \left[ 1 - \left( \frac{\rho}{R_\perp} \right)^2 - \left( \frac{z - \bar{z}_\sigma(t)}{\delta z_\sigma(t)} \right)^2 \right]^{3/2}, \]  
(6.6)
where \( R_\alpha \equiv \sqrt{2 \alpha^{-1} m \omega_\alpha^2} \) is the TF radius along the \( \alpha \)-axis and \( \epsilon_F^0 = (\omega_\perp^2 \omega_z)/(3N)^{1/3} \) is the chemical potential of an ideal two-component Fermi gas \((N_\uparrow = N_\downarrow = N/2)\). This ansatz allows for a time-dependent center-of-mass \( \bar{z}_\sigma \) and for possible axial compression when the clouds collide. The continuity equation (6.2) leads to the velocity field \( v_\sigma = v_{\sigma z} \hat{z} \) with \( v_{\sigma z}(z,t) = \dot{\bar{z}}_\sigma - \dot{\bar{z}}_\sigma \delta z_\sigma/\delta z_\sigma + z \delta \sigma/\delta z_\sigma \). Axial and radial symmetry lets us set \( \bar{z}_\uparrow \equiv \bar{z} = -\bar{z}_\downarrow \) and \( \delta z_\uparrow = \delta z_\downarrow \equiv \delta z \). Using Eq. (6.6) in (6.4) and (6.5) gives the coupled nonlinear integro-
Figure 6.2: Time dependence of the center-of-mass positions $\bar{z}_\sigma$ of the two spin clouds at unitarity for an initial separation $\bar{z}_\uparrow(t=0) = R_z$, $\bar{z}_\downarrow(t=0) = -R_z$ using the upper branch energy functional and damping $\tilde{\gamma} = 1$. Red (upper) and blue (lower) curves denote the different spin species.

differential equations

$$\left( \frac{d^2}{dt^2} + \omega_z^2 \right) \bar{z}(t) = -\frac{1}{mN_\uparrow} \int d^3r \frac{\partial E}{\partial n_\uparrow} \frac{\partial n_\uparrow}{\partial \bar{z}} - \langle \gamma v_\uparrow \rangle_\uparrow, \quad (6.7)$$

and

$$\left( \frac{d^2}{dt^2} + \omega_z^2 \right) \delta z(t) = -\frac{8}{mN_\uparrow} \int d^3r \frac{\partial E}{\partial n_\uparrow} \frac{\partial n_\uparrow}{\partial \delta z} - \frac{8}{\delta z} \langle (z-\bar{z}(t)) \gamma v_\uparrow \rangle_\uparrow. \quad (6.8)$$

As a simple approximation to the counterflow damping [100, 101] at unitarity, we choose

$$\gamma = \tilde{\gamma} \sqrt{\epsilon_{F\uparrow} \epsilon_{F\downarrow}}, \quad (6.9)$$

where the dimensionless $\tilde{\gamma}$ is of order unity and $\epsilon_{F\sigma}(r) = (6\pi^2 n_\sigma(r, t))^{2/3}/2m$ is the local Fermi energy of the $\sigma$-component. This form of $\gamma$ ensures that counterflow damping only occurs where the two spin species overlap.

6.1.2 Energy Functional

To solve these equations, we now need to specify the energy functional $E[n_\sigma]$ relevant for dynamics on the time scale $\tau_2 \ll t \ll \tau_3$. The ground state (“lower branch” of the Feshbach resonance) for $a_s > 0$ must necessarily involve bound pairs, but since $t \ll \tau_3$, the three-body processes required for the system to relax to this state have not yet occurred. However, for $\tau_2 \ll t$, the system develops short-range, two-body correlations characteristic of the metastable “upper branch” state, which was studied theoretically in Refs. [36, 37, 103], motivated by an earlier experiment [35]. The notion of the upper branch comes from the
two-body problem (either in a finite box or in a harmonic potential), where it is completely well-defined for all values of $a_s$, positive or negative. The two-body wavefunction in the upper branch is a scattering state with a single node that makes it orthogonal to the ground state (lower branch) wavefunction. Generalizing to the many-body case [36, 37], we assume that the total energy is most sensitive to these short-range correlations. The conditions that must be satisfied are [36]:

1. The many-body wavefunction includes, apart from the nodes introduced by the Pauli principle, one additional node for any pair of fermions with opposite spin.
2. The wavefunction should reduce, in the limit of the two-body problem, to that of the scattering states with one node in the relative wavefunction.
3. The energy of the system must be larger than that of the non-interacting Fermi gas, and it should reduce to the perturbative result in the weakly interacting regime $0 < k_F a_s \ll 1$.

We emphasize that orthogonality with the many-body ground state (of the BEC-BCS crossover) is not sufficient to enforce the upper branch.

We take the many-body wavefunction in the upper branch to be of the Jastrow-Slater form

$$
\Psi = \left[ \prod_{i,j} f(|r_i| - |r_j|) \right] \Phi_S(\{r_{i\uparrow}\}) \Phi_S(\{r_{j\downarrow}\}),
$$

(6.10)

where $\Phi_S(\{r_{\sigma}\})$’s are Slater determinants for spin $\sigma$ fermions and the Jastrow factor $f(r)$ describes the short-range correlations between fermions. The effective repulsion between between up and down spins in the upper branch is crucially related to the node in $f(r)$, in contrast to the node-less Jastrow factor for the lower branch. For small $a_s > 0$, the node occurs at $a_s$, with $f(r) \sim (1 - a_s/r)$ similar to the two-body problem. For larger $a_s$, the position of the node saturates [36] to $\sim 1/k_F$, the only length scale at unitarity. The main result of the QMC studies [36, 37] of the upper-branch wavefunction, Eq. (6.10) is that the system undergoes phase separation when interactions are sufficiently strong, $k_F a_s > 1$. We prefer to call this phase separation, rather than ferromagnetism, since both $N_{\uparrow}$ and $N_{\downarrow}$ are conserved and there is neither broken spin-rotational nor broken time-reversal symmetry.

We need $E[n_\sigma]$ for arbitrary polarization, which has not been studied by QMC. We use a simple approximation, the LOCV method [104, 105], which has been used for the upper branch thermodynamics [106] and is in close agreement with QMC [36, 37]. Hydrodynamics requires $T > 0.1\epsilon_F$ [96, 97] however, for simplicity, we use the zero temperature LOCV energy functional to study the dynamics. We expect that it will qualitatively describe the physics at low temperatures. The energy, then, of the Jastrow-Slater state is given by

$$
E = \frac{3}{5} \epsilon_F n + \frac{n^2}{4} \int d^3 r f^*(r) \left[ -\frac{\nabla^2}{m} + v(r) \right] f(r),
$$

(6.11)
where \( v(r) \) is the short-range two-body potential, \( n = n_\uparrow + n_\downarrow \) is the total density, and 
\[ \varepsilon_F = \frac{(3\pi^2 n)}{2m} \]

is the Fermi energy. The effect of a zero-range contact potential may be written in terms of the Bethe-Peierls boundary condition 
\[ \lim_{r \to 0} (rf(r))'/(rf(r)) = -1/a_s. \]

In addition, within LOCV, the Jastrow function \( f(r) \) satisfies the following conditions: 
\[ f(r \geq d) = 1 \text{ and } f'(d) = 0. \]

The “healing length” \( d \) in turn is defined so that 
\[ 2\pi n \int_0^d dr r^2 f^2(r) = 1. \]  
(6.12)

Variation of the energy (6.11) with respect to \( f(r) \), while taking into account the constraint (6.12) by a Lagrange multiplier \( \lambda \), gives us the “Schrödinger” equation 
\[ \left[-\frac{\nabla^2}{m} + v(r)\right] f(r) = \lambda f(r). \]  
(6.13)

Retaining only the \( s \)-wave part of this equation, we find the general solution with one node is given by 
\[ f(r) = \frac{d \sin(\kappa(r - b))}{r \sin(\kappa(d - b))}, \]  
(6.14)

where \( \kappa = \sqrt{m\lambda} \). We find that \( f(d) = 1 \) and \( f'(d) = 0 \) lead to \( \kappa d = \tan(\kappa(d - b)) \) and the Bethe-Peierls boundary condition gives \( \kappa a_s = \tan \kappa b \). With the normalization condition (6.12), we can solve for \( \kappa, d \) and \( b \) for each value of scattering length \( a_s \). The energy of the system is given simply by 
\[ \mathcal{E} = \frac{3}{5} \varepsilon_F n + \frac{1}{2} n \lambda. \]  
(6.15)

In the case of our interest, however, the system is not necessarily balanced, so that \( x \equiv n_\downarrow /n_\uparrow \) need not be unity. We have to extend the LOCV calculation to the spin-imbalanced case in which the Slater determinants will have different sizes. We find the energy of the system is given by 
\[ \mathcal{E} = \frac{3}{5} \varepsilon_F n_\uparrow \left(1 + x^2\right) + n_\uparrow n_\downarrow \int d^3 r f^*(r) \left[-\frac{\nabla^2}{m} + v(r)\right] f(r). \]  
(6.16)

Now, in general, there is no unique way to enforce the normalization conditions as in (6.12). A natural extension is to use both normalizations 
\[ 4\pi (n - n_\sigma) \int_0^{d_\sigma} dr r^2 f_\sigma^2(r) = 1, \]  
(6.17)

which introduces two healing lengths, \( d_\uparrow \) and \( d_\downarrow \). Accordingly, we shall introduce two
Lagrange multipliers $\lambda_\uparrow$ and $\lambda_\downarrow$ and the energy of the system can then be written as

$$\mathcal{E} = \frac{3}{5} \epsilon_F \mathcal{N}_\uparrow + \frac{3}{5} \epsilon_F \mathcal{N}_\downarrow + \frac{1}{2} (n_\uparrow \lambda_\downarrow + n_\downarrow \lambda_\uparrow).$$  \hfill (6.18)

In Fig. 6.3 (a), we show the upper branch energy as a function of polarization $P \equiv (1 - x)/(1 + x)$ for various values of $k_F a_s$. For small $k_F a_s$ (in fact, $k_F a_s < 0.91$), the minimum energy is attained at $P = 0$. For larger values, $k_F a_s \geq 1.124$, the minimum value is attained at $P = 1$. For intermediate values of $k_F a_s$, the minimum value occurs at a value of $0 < P_c < 1$. In Fig. 6.3 (b), we show the upper branch energy as a function of $1/k_F a_s$ for various values of the polarization $P$. Note that for $P = 1$, i.e., completely polarized, the energy is completely flat, since there is no interaction between the polarized fermions.

In Fig. 6.3 (c), we show the phase diagram of the system as obtained from LOCV. For $1/(k_F a_s) > 1.124$, the system is a homogeneous mixture of the two hyperfine-Zeeman states. We call this a Fermi liquid (FL) state. For $1.124 > 1/(k_F a_s) > 0.91$, the system is in the partially polarized phase (PP). Here the transition as predicted by the LOCV method is second order and accompanied by a divergent spin susceptibility [106]. Note that the value of $1/(k_F a_s)$ at the transition is very close to that predicted by QMC calculations [36, 37] and compares favorably with the calculation in Ref. [107]. Lastly, for $1/(k_F a_s) < 0.91$, the system is a fully polarized, non-interacting Fermi gas.
Figure 6.4: (Color online) Time dependence of the center-of-mass positions $\bar{z}_\sigma$ of the two spin clouds for $k_F(0)a_s = 2$.

### 6.2 Dynamics at unitarity

We solve Eq. (6.7) and Eq. (6.8), using (6.18) with densities $n_\sigma(r,t)$ given by Eq. (6.6). For the damping, we use Eq. (6.9) with $\gamma = 1$ and an $\epsilon_F$ corresponding to $N = 7.5 \times 10^5$ atoms and a trap anisotropy $\omega_\perp = 10\omega_z$. As our initial conditions, we take the two clouds to be displaced from the trap center by the axial TF radius, $\bar{z}_\uparrow(t = 0) = R_z, \bar{z}_\downarrow(t = 0) = -R_z$ with initial axial width $\delta z(0) = R_z$ equal to its equilibrium value.

The results at unitarity are shown in Fig. 6.2. The two clouds bounce off each other for several oscillations due to the repulsive nature of the upper branch functional. The period of the initial bounce is roughly $0.56(2\pi/\omega_z)$, slightly less than the experimental value $0.61(2\pi/\omega_z)$ [6]. We attribute this difference to the simple TF ansatz (6.6) used to model the dynamics. The bounce persists for several cycles in spite of the very large damping ($\epsilon_F^0/\omega_z \gg 1$), because the overlap between the two clouds is quite small. Once the oscillation is damped out, the two clouds remain segregated, with a final $(\bar{z}_\uparrow - \bar{z}_\downarrow)$ approximately 0.4 times the initial separation. This intermediate time behavior reflects the tendency to phase segregate in the upper branch at unitarity. The long time behavior, not described here, will be dominated by spin diffusion and three-body processes.

While the gas behaves hydrodynamically in the overlap region, most of the atoms in the opposing clouds never come into contact with each other (as a result of the bounce) and are essentially non-interacting. Nonetheless, the crucial physics that produces the bounce arises in the overlap region where hydrodynamics is valid. Moreover, due to Pauli repulsion, the motion of the gas in the non-overlap regions is essentially a rigid-body dipole oscillation, insensitive to the choice of a collisional (hydrodynamic) or collisionless theory.
6.3 Collisional dynamics away from unitarity

Away from unitarity, it may be harder to reach the hydrodynamic regime. If $\omega_z$ is sufficiently small, however, it will always be the case that the dynamics in this direction are hydrodynamic. The greater challenge at finite $a_s > 0$ is that $\tau_3$ may not be much greater than $\tau_2$. As $a_s$ decreases from unitarity, one expects that $\tau_3$ reaches a minimum for $k_Fa_s \sim 1$ and then becomes large again [28], with $\tau_3 \sim (na_s^3)^{-2}\frac{1}{\sqrt{\epsilon_F}}$ for $k_Fa_s \ll 1$. In contrast, the cross-section $a_s^2$ determines $\tau_2 \sim (na_s^3)^{-2/3}\frac{1}{\sqrt{\epsilon_F}}$. Hence, for small $k_Fa_s$, again $\tau_3 \gg \tau_2$.

However, when $k_Fa_s \sim 1$, it is conceivable that $\tau_3 \sim \tau_2$.

With these caveats in mind, we solve our hydrodynamic equations away from unitarity to better understand the relationship between the intermediate-time dynamics, after the bounce is damped out, and the upper branch equation of state: Fermi liquid ($k_Fa_s < 1$) versus phase separated ($k_Fa_s > 1$). The solutions of (6.7) and (6.8) at $k_F(0)a_s = 2$ and 0.5 (using the same initial conditions and $\epsilon_0^\prime$ as in Fig. 6.2), are shown in Figs. 6.4 and 6.5. Here $k_F(0) = \sqrt{2m\epsilon_F}$ is the Fermi wavevector of an ideal gas at the trap center. To simplify the numerical work, we use the mean-field energy functional $E = 4\pi a_s n_1 n_1/m$ in place of the LOCV result. In addition, we use a microscopic expression for the damping, obtained from a relaxation-time approximation to kinetic theory (see Eq. (20) in Ref. [100]). Symmetrizing in the spin components, as in (6.9), we write $\gamma = (4/9\pi)(\sqrt{k_{F\uparrow}k_{F\downarrow}}a_s)^2\sqrt{\epsilon_{F\uparrow}\epsilon_{F\downarrow}}$.

Even at small $k_F(0)a_s$, the clouds exhibit a weak bounce due to compressional recoil, which damps out very quickly. We see, however, a clear difference between Fig. 6.4 ($k_Fa_s > 1$), where the clouds remain separated, and Fig. 6.5 ($k_Fa_s < 1$), where they merge. The details of the short-time collision dynamics at small $k_Fa_s$ may well be better modeled by a kinetic theory, rather than hydrodynamics. The longer time behavior – with a separated or mixed equilibrium state – is a robust conclusion of our theory, however, as long as the
atoms are predominantly in the upper branch. This behavior is qualitatively similar to the experimental results shown in Supplementary Fig. 1 of Ref. [6]; see below.

6.4 Discussion

We now compare our results with the experiments. As seen from Fig. 6.2, our results at unitarity – the short-time bounce, the damping of the oscillations and the separation of the clouds at intermediate times – are all in very good agreement with Ref. [6].

Away from unitarity, at finite values of $k_Fa_s > 0$, our results are qualitatively similar to the experimental data shown in Supplementary Fig. 1 of Ref. [6]. For time scales $\tau_2, \omega_z^{-1} \ll t \ll \tau_3$, say, $t = 200$ ms, the system remains phase segregated for large $k_Fa_s$ [Figs. 1(f,g)], while completely mixed for small $k_Fa_s$ [Figs. 1(c,d,e)]. In fact, a very rough estimate for the critical $k_Fa_s$ can be read off from the experimental data: It is between 0.26 [Fig. 1(e)] and 1.2 [Fig. 1(f)]. Our theory is not applicable to the long-time merging of clouds that are segregated at intermediate times. This could involve three-body collisions that relax the system to the lower branch and spin diffusion, which is always present at finite temperatures.

Finally, we comment on the experiment of Jo et al. [35] in which a spin-balanced mixture, initially at a small positive $a_s$, is swept close to resonance, thereby generating strong interactions in the upper branch. It appears, however, that rapid three-body losses render it unstable to the lower branch within a very short time interval ($\sim 5$ ms) [38, 99] and phase separated ferromagnetic domains are not observed.

In contrast, the specific initial configuration in the colliding cloud experiment [6] proves to be crucial for the (meta)stability of the upper branch. In this case, three-body loss is limited spatially within the overlap region between up and down spins at the trap center, and temporally to a fraction of the oscillation period. As such, the effective $\tau_3$ is greatly enhanced and one can study the metastable upper branch.

The experimental observation of the bounce followed by the two clouds sitting side-by-side for as long as $\sim 100$ ms validates our assumption of a long $\tau_3$. If $\tau_3$ had been very short, the system would have rapidly relaxed into the lower branch. We cannot see how a lower-branch energy functional, with attractive interactions forming bound pairs, could lead to the observed dynamics.

6.5 Conclusions

We conclude by summarizing our physical picture for the colliding spin-polarized clouds. Our main hypothesis is that fast two-body collisions ($\tau_2$) establish local thermal equilibrium in the overlap region of the clouds, while three-body processes ($\tau_3$) have not driven the system to the lower branch yet. The hydrodynamic time evolution for $\tau_2 \ll t \ll \tau_3$ is then governed by a repulsive energy functional corresponding to the upper branch of the
Feshbach resonance. The effective repulsion on the upper branch leads to the bounce, and also to the qualitative difference between the segregation of the clouds for $k_Fa_s > 1$ and their merging for $k_Fa_s < 1$, which reflects the phase transition in the upper branch equation of state [36, 37].


[Bibliography]


