BEC-BCS CROSSOVER WITH FESHBACH RESONANCE FOR THREE-HYPERFINE-SPECIES MODEL

BY

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DISSERTATION

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Abstract

The BEC-BCS crossover problem has been intensively studied both theoretically and experimentally largely thanks to Feshbach resonances which allow us to tune the effective interaction between alkali atoms. In a Feshbach resonance, the effective s-wave scattering length grows when one moves toward the resonance point, and eventually diverges at this point. There is one characteristic energy scale, δ_c, defined as, in the negative side of the resonance point, the detuning energy at which the weight of the bound state shifts from predominatedly in the open-channel to predominated in the closed-channel. When the many-body energy scale (e.g. the Fermi energy, E_F) is larger than δ_c, the closed-channel weight is significant and has to be included in the many-body theory. Furthermore, when two channels share a hyperfine species, the Pauli exclusion between fermions from two channels also needs to be taken into consideration in the many-body theory.

The current thesis addresses the above problem in detail. A set of gap equations and number equations are derived at the mean-field level. The fermionic and bosonic excitation spectra are then derived. Assuming that the uncoupled bound-state of the closed-channel in resonance is much smaller than the inter-particle distance, as well as the s-wave scattering length, a_s, we find that the basic equations in the single-channel crossover model are still valid. The correction first comes from the existing of the finite chemical potential and additional counting complication due to the closed-channel. These two corrections need to be included into the mean-field equations, i.e. the gap equations and the number equations, and be solved self-consistently. Then the correction due to the inter-channel Pauli exclusion is in the order of the ratio of the Fermi energy and the Zeeman energy difference between two channels, E_F/η, which can be analyzed perturbatively over the previous corrections.

Fermionic and bosonic excitation modes are studied. Similarly as the mean-field result, the basic structure follows that of the single-channel model, and the correction due to the inter-channel Pauli exclusion can be treated perturbatively with expansion parameter in the order of E_F/η. In the bosonic excitation, a new out-of-sync phase mode emerges for the two-component order parameters. It is nevertheless gapped at the the pair-breaking energy.

To Jie, Ethan and Chloe

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α	Ratio of the closed-channel correlation $h_{2\mathbf{k}}$ to the normalized two-body closed-channel bound state wave function, $\phi_{\mathbf{k}}$, at high momentum. $h_{2\mathbf{k}} \xrightarrow{\text{high momentum}} \alpha\phi_{\mathbf{k}}$. (Page 42)
$\gamma_{i\mathbf{k}}$	Correction of the fermionic excitation spectrum over $\pm E_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}} + \eta$. (Page 38)
δ_c	Energy scale of the detuning from resonance when the closed-channel takes substantial weight. (Page 16)
$\Delta_{1,2}$	Order parameters in the open-channel and closed-channel. (Page 33)
ζ	Small characteristic dimensionless parameter for the inter-channel Pauli exclusion, $\zeta = \frac{\Delta_2^2}{\Delta_1 \eta}$. (Page 37)
η	Absolute detuning between two channels. Note that $\eta = 0$ is not where a_s diverges. (Page 13)
κ	Momentum scale of the resonant bound state in the isolated close-channel, namely $\kappa^2/2m = E_b$.
λ_1, λ_2	Two new parameters in the renormalized gap equation for two channels. They describe the inter-channel Pauli exclusion effects between the two channels. (Eqs. 5.48 and 5.49 in Page 44 and 45)
μ	Chemical potential.
ϕ_i	Bound-state wave functions of the isolated close-channel; especially, ϕ_0 is the one at resonance. (Page 42)
a_{bg}	The background s-wave scattering length in the open-channel when it does not coupled to the closed-channel. (Page 14)
a_c	Characteristic size of the bound state at resonance (ϕ_0) if the close-channel is isolated. It is proportional to the inverse of κ.
a_s, $a_s^{(o)}$	The effective open-channel s-wave scattering length. Subscript $^{(o)}$ will be dropped when there is no ambiguity. Alternatively, it is the single parameter in the Bethe-Pierels boundary conditions. (Page 9, 15)
a_0	Average inter-particle distance, $a_0 k_F \sim 1$.
E_b, $E_b^{(i)}$	Binding energy of the i^{th} two-body (bound) eigenstate in the isolated close-channel. Superscript $^{(i)}$ is dropped when referring to the one in resonance. (Page 13)
$E_{\mathbf{k}}$	Defined as $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}$, where $\epsilon_{\mathbf{k}} = \hbar^2 k^2/2m$ is the kinetic energy. $E_{\mathbf{k}}$ corresponds the elementary fermionic excitation energy for $\mathbf{k}$ in the single channel. In the two-channel case, $E_{\mathbf{k}}$ is defined in the similar way as, $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_1^2}$, where Δ_1 is the order parameters of the open-channel. However, it is then only the zeroth order energy for the two elementary fermionic excitation modes. (Page 23)

$h_{1\mathbf{k}}$, $h_{2\mathbf{k}}$	(Open and closed)-channel anomalous two-body correlations of the many-body system. (Page 39)
k_F	Fermi momentum. $k_F = \hbar(3\pi^2 n)^{1/3}$ in 3D.
$n_{o(pen)}$	Density of the open-channel atoms.
$n_{c(lose)}$	Density of the closed-channel atoms.
$n_{tot(al)}$	Density of all atoms.
r_c	Potential extension. All potentials are taken as zero outside r_c.
$\mathcal{V}_0$	Total volume of the system.

Chapter 1

Introduction

From a methodological view, a physical system would be very desirable for developing and verifying a theory if it can be described with as few parameters as possible, and each parameter is as tunable as possible. One such system is the ultracold dilute fermionic alkali gas with the Feshbach resonance. Dilute fermionic alkali gas was cooled into degenerate region in 1999 [DeMarco and Jin, 1999]. Not long after that, superfluidity was observed for such systems in 2003 [Regal et al., 2003]. In dilute ultracold fermionic alkali gas, it is sufficient in many phenomena to describe an atom-atom interaction with one single parameter, namely the s-wave scattering length, a_s, because the gas is very dilute and experiments are performed at very low temperatures.

The other desirable property is the ability to tune the effective interaction strength, i.e., in the present case, the s-wave scattering length, a_s through Feshbach resonances. One atomic energy level splits into several hyperfine levels under a magnetic field, due to the hyperfine interaction between nuclear spins and electronic spins. Hyperfine spin indices provide a good set of quantum numbers for a single atom. In the theory of atom-atom interactions, a channel refers to a specific configuration of hyperfine spin indices of one atom pair. Different channels usually have different magnetic moments and therefore have different Zeeman energies in the presence of a magnetic field. The difference of the Zeeman energies can then be tuned by changing the magnetic field. In addition, a channel is no longer an exact eigenstate when the atom-atom interaction is taken into consideration because the interaction is mostly due to the overlap between electronic parts of the two-atoms' wave-functions. As a result, channels are hybridized. The effective potential of each channel is also different. The potential of one channel may be deep enough to sustain a bound state. This channel is then called *"closed-channel"*. For a certain magnetic field, the energy level of this bound state might be close to the zero-energy threshold of the other channel, usually called *open-channel*, and two channels thus strongly hybridized. The low-energy scattering properties in the open-channel is then dramatically modified. In such a situation, two atoms approaching each other in the open-channel may "spend a certain amount of time in the closed-channel" and then reemerge in the open-channel. Atoms in the open-channel seem to feel an enhanced effective interaction. This phenomenon is known as Feshbach resonances. We will present a quantitative analysis about alkali gas in Chpater 2 and Feshbach resonances

in two-body context in Chapter 3.

A very desirable property of the Feshbach resonance is that the effective interaction is tunable experimentally through the Zeeman energy difference between channels which is in turn tunable through instruments such as a magnetic field. This unique ability gives physicists a rare opportunity to study a many-body system under various interaction strengths, and thus connect different physics originally developed separately. Particularly for the fermionic gas, there are a series of theoretical works about uniform treatment of BEC and BCS since the 1960s [Eagles, 1969, Leggett, 1980, Nozières and Schmitt-Rink, 1985, Randeria, 1995], for which dilute ultracold fermionic alkali gas with Feshbach resonances provides the perfect testing grounds. Indeed, these theories works quite well qualitatively.

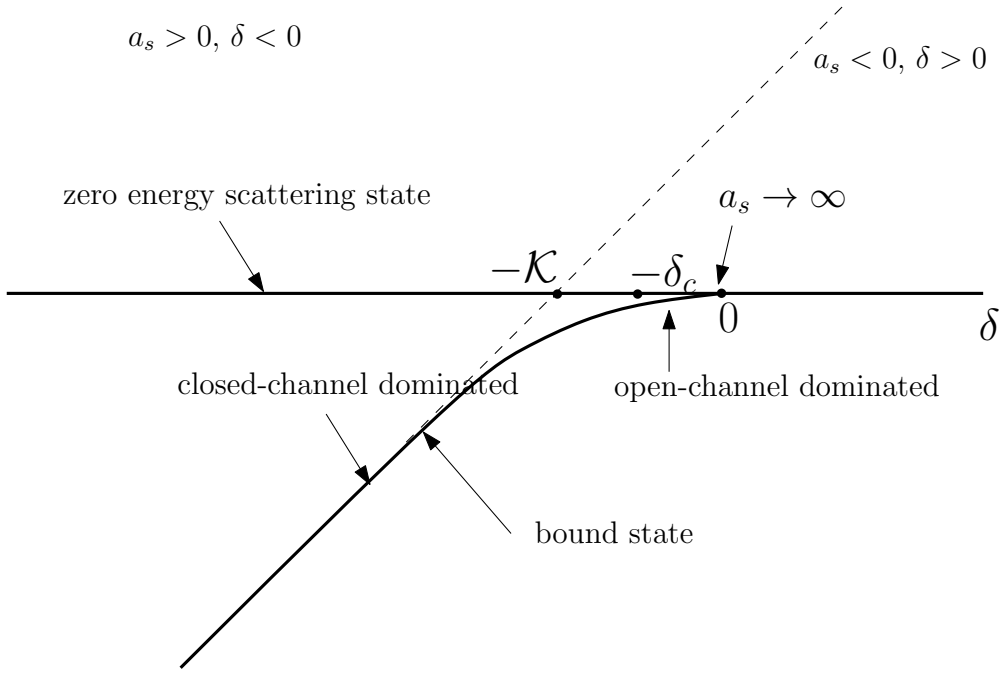


Figure 1.1: Energy levels in a Feshbach resonance
δ is the energy detuning from the resonance point, where the resonant point is defined as the point where the open-channel effective s-wave scattering length diverges, $a_s \to \pm\infty$. The horizontal line stands for the zero energy s-wave scattering state, $\psi \sim \frac{1}{r} - \frac{1}{a_s}$, which exists for any detuning. The lower line stands for the real bound state, which only exists for negative detuning ($\delta < 0$, $a_s > 0$). The dash line stands for the (uncoupled) closed-channel bound state. An interesting point to notice is that the real bound state appears earlier than the cross point of the (uncoupled) closed-channel bound state level and zero energy. Another important point to notice is the negative detuning $-\delta_c$. When the negative detuning is smaller than δ_c, this real bound state is composed mostly with atoms in the open-channel and vice verse. See Chapter 3 for details about $\mathcal{K}$ and δ_c.

The two-body theory of the Feshbach resonance has a characteristic parameter, δ_c, defined as the detuning energy at which the weight of the bound state shifts from predominated in the open-channel to predominated

in the closed-channel (see Fig. 1.1). Naïvely speaking, in the negative detuning side of any resonance (i.e. $\delta < 0$), particles should mostly stay in a (virtual) bound-state of the closed-channel (or "virtual state" in some other resonances). However, at the resonance point of the Feshbach resonance ($a_s \to \pm\infty$), atoms are mostly still in the open-channel, and they do so down to a negative detuning $\delta \sim -\delta_c$. Only when the detuning from resonance is much far away than δ_c, do atoms have the majority weight in the closed-channel.

When considering a many-body problem, an important question is how this energy scale, δ_c, compares to a typical many-body energy scale, namely, the Fermi energy of the free fermionic atoms. In the region not too far away from resonance ($|\delta| \ll \delta_c$), the closed-channel weight is negligible if the Fermi energy is much smaller than δ_c, (i.e., *broad resonance*). Crossover experiments are usually performed at detuning not too far from the resonance, and hence the closed-channel can be safely ignored at the many-body level. Eventually, when the detuning is too far away, $|\delta| \gg \delta_c$, the bound state is almost like the uncoupled closed-channel bound state with a little dressing from the open-channel. We nevertheless do not concern such cases for the broad resonance because crossover phenomena have already be well covered in both BEC and BCS ends with $|\delta| \ll \delta_c$. The problem can be well-described as a two-species fermion system with a tunable interaction. The Feshbach resonance indeed serves as a simple "magic" knob to change the interaction strength. The original theories developed on single-channel models apply to this case directly. This is also the situation for two popular experiment cases (^{6}Li atoms at 834G, ^{40}K atoms at 224G). Many theoretical works have been developed using the single-channel model as these original works or using the tow-channel model within the broad resonance assumption (e.g. [Holland et al., 2001, Ho, 2004, Fuchs et al., 2004]). On the contrary, when the Fermi energy of the free fermionic atoms is comparable to or even larger than δ_c, the closed-channel has to be included at the many-body level even for small detuning. Such a situation, previously considered in some works [Gurarie and Radzihovsky, 2007], is the focus of the current thesis.

Nevertheless, one crucial simplification comes from the fact that relevant uncoupled closed-channel bound state is tightly bound, with spatial extension much smaller than many-body scales, e.g. the interparticle distance, (but often larger than the potential range). This fact enable us to treat the Pauli exclusion between two channels perturbatively. It is not necessary to handle all the fermion species simultaneously, which probably requires quite different techniques other than those discussed in this thesis.

To complicate the problem even further, real experimental configurations often have one common hyperfine species between the two channels. There are three hyperfine species in the two channels instead of four species (two for each channel). Two most common setups (^{6}Li at 834G, ^{40}K at 224G) both contain three species of fermions although they are the broad resonance. The Pauli exclusion principle prevents atoms of both channels from occupying the same level simultaneously because of this common species. The

inter-channel Pauli exclusion has no counterpart in two-body physics. This peculiar effect in many-body crossover problems has received little theoretical attention up to now. Nevertheless, narrow resonances do exist [Chin et al., 2010] and it is not inconceivable to perform many-body experiments using such resonances. The central concern of this thesis is about these situations.

Roughly speaking, turning from two-body systems to many-body systems brings three effects into the original two-body problem. The first effect is closely associated with the Fermi energy: For a many-body fermionic system at low temperature, most fermions are inactive; only the fermions close to the Fermi surface participate in the interaction processes. Therefore, energy often needs to be measured from the Fermi surface instead of from zero as in a two-body situation. This aspect has been extensively studied previously [Gurarie and Radzihovsky, 2007].

The second effect is about counting. Unlike in the single-channel problem, there are two relevant densities in the two-channel problem: the density of atoms in the open-channel, n_o, and the density of atoms in the closed-channel, n_c. When the closed-channel weight is small (broad resonance), it is all right to treat the total density as the same as the open-channel density. However, in the narrow resonance, where the closed-channel weight is not negligible, counting becomes complicated. Extra care is required to specify which channel the quantities, such as "density", belong to. This aspect has been also extensively studied previously [Gurarie and Radzihovsky, 2007].

The last effect is unique for the three-species problem, where one common species is shared by both channels. The phase spaces of two channels are overlapped because of the Pauli exclusion caused by the common species. This effect is controlled by the wave-function overlapping of states in the two channels. A rough estimate of this overlapping can be made: The uncoupled closed-channel bound-state which is in resonance with the open-channel zero energy threshold has relatively small spatial extension, a_c. Its binding energy E_b is close to the Zeeman energy difference between two channels, η. On the other hand, fermions in the open-channel fill the lowest momentum states up to typically the Fermi energy, E_F. By a simple dimensional argument, the ratio E_F/η must control the overlapping effect. This effect has not been addressed in any theoretical work to this author's knowledge. How it modifies the many-body picture is the central topic of this thesis.

We can see this from a slightly alternative aspect using two-fermion molecule gas for the uncoupled closed-channel bound state. We assume that the molecule size is a_c and the total number of molecules is N. Assuming further that the bound-state is close to threshold, the bound-state wave function can then be written as $A/(k^2+\kappa^2)$, where $\hbar^2\kappa^2/2m = E_b$, (see Appendix B.3). The prefactor "A" can be determined by normalization, $\sum_{k=0}^{1/a_c} |\psi|^2 \sim N$. Now we consider all atoms in a typical many-body scale, e.g. the Fermi

energy, E_F, which is going to overlap with levels occupied in the open-channel. Usually, the Fermi energy is much smaller than the energy scale of the closed-channel bound state, $E_F \ll E_b$. The total number of atoms in $[0, E_F]$ is roughly $N \cdot (k_F a_c)^3$, which is much smaller than N. This means that in the two-channel problem, the low momenta, ($k \lesssim k_F$), are still dominated by the open-channel component even when the total number of atoms in the closed-channel is comparable or higher than the total number of atoms in the open-channel because atoms in the closed-channel are mostly in high-momentum states.

The present thesis is divided as follows: Chapter 2 to 4 review several important concepts used in the thesis. Chapters 5 and 6 then present my main work and Appendix A lists an earlier attempt using a roughly equivalent but less-flexible approach.

More specifically, Chapter 2 briefly reviews dilute ultracold alkali gas. Section 2.3 in particular examines the idea of "universality", which is one of the central ideas in our treatment of the two-channel model. Chapter 3 goes over the Feshbach resonance in two-body physics and the concept of the narrow (broad) resonance is introduced. Chapter 4 reviews the single-channel BEC-BCS crossover problem as well as the path-integral approach solving it. This chapter serves as the starting point for the solution of the two-channel model. After these reviews, Chapter 5 and Chapter 6 present my work on the three-species narrow Feshbach resonance within a many-body path-integral framework, in detail. Chapter 5 discusses the mean field result while Chapter 6 discusses fermionic and bosonic excitations. An earlier attempt based on the BCS ansatz approach in mean-field level is given in Appendix A. Chapter 7 discusses our procedures and their conclusions.

Chapter 2

Dilute ultracold alkali gas

Since the 1990s, dilute alkali gas has been cooled into quantum degenerate region where the thermal de Broglie wavelength ($\frac{h}{\sqrt{2\pi m k_B T}}$) is comparable or larger than the interparticle distance. Not long after successfully cooling the bosonic atoms, fermionic alkali gas was also available in the degenerate region. Because of the ultra-low temperature (in the order of nK), and the extreme diluteness ($10^{12} \sim 10^{15}\text{cm}^{-3}$), the atoms are mostly *free* except when they are close. This particular property simplifies theoretical analyses tremendously (see Sec. 2.3 for details). In this chapter, we review a few aspects of the dilute ultracold alkali gas that are closely related to the current thesis.

2.1 A single atom and its hyperfine levels

In experiments on ultracold alkali gas, a magnetic field ($\mathbf{B}$) is the most common physical quantity to manipulate. Let us first study an isolated atom in the presence of a magnetic field. An alkali atom has only one electron in its outer shell. All the rest electrons are in the filled inner shells which has no total magnetic moment. So we only need to consider the spin of the outermost electron, $\mathbf{S}$, for interaction with the magnetic field. In addition, a magnetic field also interacts with the atom's nuclear spin, $\mathbf{I}$. The full spin-part Hamiltonian is

$$\begin{aligned} H_{spin} &= A\mathbf{I}\cdot\mathbf{S} - \mu_e \mathbf{B}\cdot\mathbf{S} - \mu_n \mathbf{B}\cdot\mathbf{I} \\ &= A\mathbf{I}\cdot\mathbf{S} - \mu_e B S_z - \mu_n B I_z \end{aligned} \tag{2.1}$$

The first term with a characteristic energy A describes the hyperfine interaction, while the next two terms describe Zeeman energies of the outer electron and nuclei respectively. μ_e is the electronic magnetic moment, while μ_n is the nuclear magnetic moment. In the second line, we take the direction of the magnetic field as the z-direction. This Hamiltonian can be diagonalized by introducing the total spin

$$\mathbf{F} = \mathbf{S} + \mathbf{I} \tag{2.2}$$

When the magnetic field is zero, the two Zeeman energy terms in the above Hamiltonian vanish. Thus, (F, F_z) are good quantum numbers and all states with the same F are degenerate. When the magnetic field is finite, (F, F_z) cannot diagonalize the Zeeman energy terms, and therefore are no longer good quantum numbers. Nevertheless, we can still label the atomic states with these two numbers via the adiabatic connection to the levels in the zero magnetic field. For a finite magnetic field, except for states with the highest and lowest F_z, namely, $\pm F$, each other state is a mixture of different (S_z, I_z) or (F, F_z). Fortunately, S is just equal to $1/2$ for an alkali atom. So each state is mixed with at most two sets of quantum numbers (S_z, I_z). At high magnetic fields, the first hyperfine coupling term in Eq. (2.1) is dominated by the last two terms of Zeeman energies and the eigenstates are approximately described by the quantum numbers (S_z, I_z). (See Fig. 2.1.)

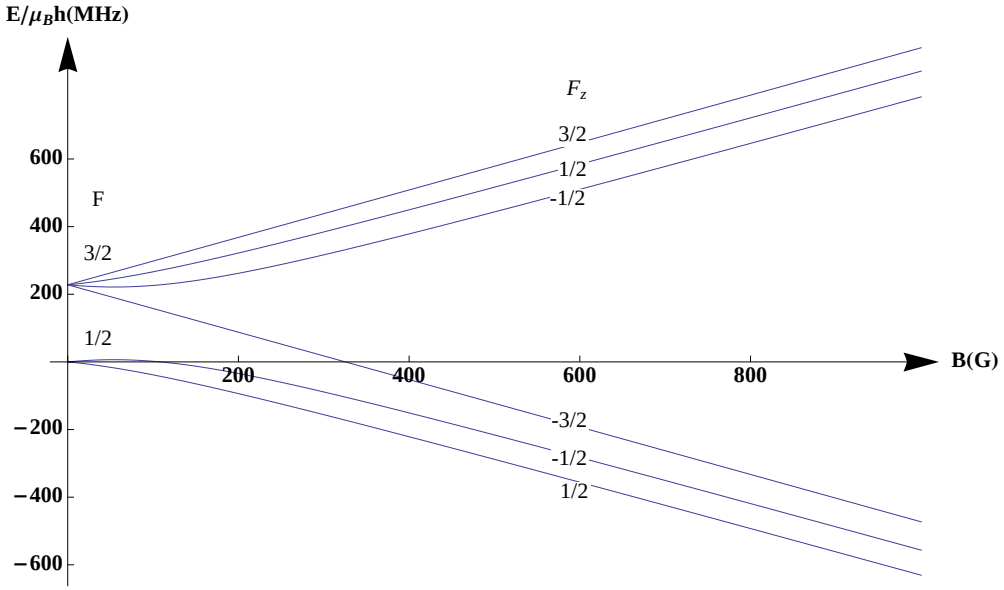


Figure 2.1: Hyperfine structure of a single ^{6}Li atom
Levels are marked with F and F_z (see Footnote 1 in page 7)

2.2 Two-body interactions

Things would be very boring if there was only the single-atom Hamiltonian. Before discussing the interaction itself, let us introduce one important concept related to it. The term "channel" is used to refer one configuration of hyperfine spins for one atom pair in interaction, $\left|F^{(1)}, F_z^{(1)}\right\rangle \otimes \left|F^{(2)}, F_z^{(2)}\right\rangle$. [1] Channels are good basis for non-interaction pairs. A pair of atoms in one channel would stay in this channel forever in the absence of interactions between atoms. Considering the present case of alkali atoms, two alkali atoms

[1] Remember that (F, F_z) are only labels; they do not stand for the total angular momentum unless there is no magnetic field.

mostly interact through the overlapping of their electron wave-functions in the dilute limit. Thus, besides the atom-atom distance, the interaction is mostly a function of electronic spins, with negligible dependence on nuclear spins. Schematically the interaction can be written as

$$V = f(r) + g(r)\mathbf{S_1} \cdot \mathbf{S_2} \tag{2.3}$$

Here the spatial part of the interaction is coupled with electronic spins. The hyperfine levels that diagonalize the single atom Hamiltonian are no longer eigenstates for this interaction. In another word, the interaction has non-diagonal terms between channels and therefore hybridizes them. Instead, states with definite electronic spins form a good approximate basis for the atom-atom interaction. Nonetheless, most experiments are performed in the so-called high-field region, where the Zeeman energy terms dominate the hyperfine interaction term in the single-atom Hamiltonian (Eq. 2.1). Recalling that one hyperfine state is at most mixture of the two (S_z, I_z) states. In the high-field, one of them always dominate the other; therefore the electronic spin S_z is approximately a good quantum number for a hyperfine level, and the original hyperfine levels (channels) serve as a good starting point as the zeroth order approximation. When the hybridization is taken into account, multichannel scatterings are possible. The most interesting thing in these multi-channel scatterings is the possibility of a resonance. One of them is the so-called Feshbach resonance: The potential in one channel may be deep enough to sustain a bound-state. This channel is named "closed-channel". When this bound-state energy is close to the zero-energy threshold of another channel, named "open-channel", the low-energy scattering properties in the open-channel are dramatically modified. This resonance turns out to be extremely useful in cold atom experiments. Chapter 3 reviews its theory for a two-body system. The more involving many-body problem is then the central theme of this thesis and is discussed in Chapter 5 and 6 in detail.

Let us illustrate above discussion in one example. In a common experimental setup for ^{6}Li (Fig. 2.1), experiments are usually prepared with atoms in the two lowest hyperfine levels: described by the direct product of two states, $\left|F = \frac{1}{2}, F_z = -\frac{1}{2}\right\rangle \otimes \left|F = \frac{1}{2}, F_z = +\frac{1}{2}\right\rangle$. This is a good approximation until the two atoms are very close. Recalling that the atom-atom interaction (Eq. 2.3) conserves the z-component of the total angular momentum, $F_z^{(1)} + F_z^{(2)}$, this channel mixes with four other possible channels of the same total z-direction angular momentum, i.e. $F_z^{(1)} + F_z^{(2)} = 0$: $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle \otimes \left|\frac{3}{2}, +\frac{1}{2}\right\rangle$, $\left|\frac{3}{2}, -\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2}, +\frac{1}{2}\right\rangle$, $\left|\frac{3}{2}, +\frac{3}{2}\right\rangle \otimes \left|\frac{3}{2}, -\frac{3}{2}\right\rangle$, $\left|\frac{3}{2}, +\frac{1}{2}\right\rangle \otimes \left|\frac{3}{2}, -\frac{1}{2}\right\rangle$ (All states are labeled as $|F, F_z\rangle$). Various resonances can take place. Note that close to the resonance, it is normally sufficient to consider only the channel that is in resonance, while neglect all other channels. Another important aspect is whether the two channels share one single hyperfine species or

not. In the former case, totally three hyperfine species are involved while in the later case, four hyperfine species are involved. The closed channel in the most studied resonance with a magnetic filed close 834G, is approximately $\left|\frac{3}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle$ and the resonance is a three-species resonance [Zhang, 2009, Chin et al., 2010].

2.3 Universality, Bethe-Peierls boundary conditions, the s-wave scattering length, and two-body density matrices

One important aspect of the interaction in dilute ultracold alkali gas is that for many purposes, it is sufficient to characterize the interaction by a single two-body parameter, namely, the s-wave scattering length, a_s, because both the density and the temperature, are very low. This is often interpreted as we can replace the real potential with a pseudo potential, $U(\mathbf{r}) = \frac{4\pi a_s \hbar^2}{m}\delta(\mathbf{r})$ [Pethick and Smith, 2001, Leggett, 2001]. Nevertheless, an alternative interpretation of a_s [Leggett, 2001, Tan, 2008a, Tan, 2008b, Combescot et al., 2009] is more useful in this work. For a short-range potential, where the potential range, r_c, is much smaller than the average interparticle distance, a_0, particles are free-like in the majority of the time. They only interact when two particles are close to each other. We can thus schematically divide the space into two domains: $\mathcal{D}$, where any two particles are more than r_c away from each other; and otherwise, $\mathcal{I}$. Most physical quantities would be very easy to calculate if only considering the free part, $\mathcal{D}$. In a low-energy (ultracold) dilute system, we only need to consider pair-wise interaction while neglect all the three-body or more-body interactions. In addition, $\mathcal{D}$ takes the majority of the space due to the same reason. The effect of the potential on wave-function in the short-range region, $\mathcal{I}$, can be taken simply as a boundary condition on the wave-function in the free part $\mathcal{D}$, $\psi(r) \xrightarrow{r\to 0} \psi_0(r)$. For an isometric $\psi_0(r)$, the lowest order in the radial coordinate r is $\frac{1}{r}$. [2] Including the next order, a constant, we have $\psi_0(r) \propto \frac{1}{r} - \frac{1}{a_s}$ barring the normalization. All these consideration gives us the simplest non-trivial boundary condition on a wave function

$$\psi(r) \xrightarrow{r\to 0} A\left(\frac{1}{r} - \frac{1}{a_s}\right) \tag{2.4}$$

which is also known as the Bethe-Peierls boundary condition [Bethe and Peierls, 1935]. a_s is fully determined by two-body physics. This simple boundary condition applies to two-body, few-body, as well as many-body systems, and has been proved to be a very powerful tool in solving various problems.

Eq. 2.4 coincides the zero-energy s-wave scattering wave function, which explains the name of parameter

[2] The extra $\frac{1}{r}$ factor is there for radial wave function in 3D.

"a_s", the s-wave scattering length. Nevertheless, we did not mention anything about zero energy so far, although a_s is defined for zero energy in the scattering theory context. In fact, this boundary condition (Eq. 2.4) applies generally to any low (positive or negative) energy solutions as long as the energy involved is much lower than the energy scale in the interaction domain $\mathcal{I}$. Hence, this boundary condition applys to close-to-threshold bound states as well. The s-wave wave function of a weak bound-state reads $\psi(r) = \frac{1}{r}e^{-r/a_s}$ in $\mathcal{D}$, which matches the Bethe-Peierls boundary condition with a positive a_s for $r \ll a_s$. The exponential decay factor of the wave function, a_s, is directly related to the binding energy, E_b, with the often cited relation.

$$E_b = \frac{\hbar^2}{2m_r a_s^2} \tag{2.5}$$

Here m_r is the reduced mass for center of mass, which is equal to half of the atom mass for a pair of the same atoms. This immediately clears one often confusing and counter-intuitive fact, that a positive a_s is associated to a bound state. In the standard scattering theory, a positive a_s is usually associated with a repulsive interaction, which obviously does not support a bound state.[3]

Eq. 2.4, does not fix the normalization on the wave function. This normalization factor, encapsulating effects from particles outside the immediate interacting pair, appears in many physical quantities. In a dilute and low-energy system, its square is proportional to the so-called *integrated contact intensity*, C, introduced by Tan [Tan, 2008a, Tan, 2008b, Combescot et al., 2009]. For the limit $r_c \to 0$, the integrated contact intensity, C, and the s-wave scattering length, a_s, are sufficient to describe several important physical quantities, such as internal energy. A particular useful one for this thesis is the limit at high-momentum of the particle number distribution of particles,

$$\lim_{k\to\infty} n_k = \frac{C}{k^4} \tag{2.6}$$

Note that here *high-momentum* does not mean the absolutely high-momentum, it means lower than the characteristic momentum of potential $1/r_c$, but higher than any other scale, $1/a_0$,... Indeed, when the short-range approximation and low-energy approximation apply, we expect that the two-body correlation at high-momentum ($\gg k_F$) does not change much from a two-body system to a many-body system. In this high-momentum region, we can always use the two-body wave function as good approximation.

In many-body physics, various physical observable quantities are related to one set of quantities, namely,

[3]This seeming paradox can be resolved carefully within scattering theory as follows. In the scattering theory, only when the interaction is weak, and phase shift as well as a_s are small, we have the fact that a repulsive interaction leads to a positive phase shift and a positive a_s; while an attractive interaction leads to a negative phase shift and a negative a_s. No simple relationship of signs holds for a strong interaction, where a bound state might form. In fact, the phase shift changes as much as 2π when a bound state starts to form; therefore, a_s is large and changes sign over the threshold.

density matrices, $\left\langle \Psi^\dagger(x_1)\cdots\Psi^\dagger(x_N)\Psi(x'_N)\cdots\Psi(x'_1)\right\rangle$. In fermionic system, the one-body density matrix ($N=1$) for an interacting system is often very close to the one for the free particles, although the difference can be important for some theories, such as Landau Fermi liquid theory. A two-body density matrix ($N=2$) is often used because it is often different from the two-body density matrices of the free fermions qualitatively, such as in the case of BCS pairing. Formally, we can decompose a two-body density matrix into an orthogonal basis

$$\left\langle \Psi^\dagger(x_1)\Psi^\dagger(x_2)\Psi(y_2)\Psi(y_1)\right\rangle = \sum_n C_n \phi_n^\dagger(x_1,x_2)\phi_n(y_1,y_2) \tag{2.7}$$

When one or a few C_n are macroscopic, some special quantum phenomena often emerges. Especially when only one parameter, C_0, is macroscopic, the system can often be interpreted as one macroscopic wave function, $\phi_0(x_1,x_2)$, (which is often called order parameters). [Leggett, 2006] This can serve as a starting point for several phenomena, such as BCS superconducting,...

Zhang and Leggett developed independently another universality theory based on two-body density matrices [Zhang and Leggett, 2009], which actually take a more general form of boundary conditions than the Bethe-Peierls boundary condition with a_s. They asserted that for a short-range potential and a low temperature, as in the case of dilute ultracold alkali gas, the basis wave functions ϕ_n in Eq. (2.7) follows the two-body wave function at short-range. This is actually similar to Eq. (2.4). Instead of requiring the simplest form of ψ_0 given in Eq. (2.4), they require a more general wave-function that solves the Hamiltonian at two-body level. Not surprisingly, many physical properties are determined by the normalization factors as using the Bethe-Peierls boundary condition.

In this thesis, similar idea is used. We assume that the closed-channel correlations follow the its two-body bound-state wave-function at high energy (i.e. short-range). An open-channel correlation follows its two-body wave-function at short-range, but its intermediate range does not do so because of the sensitive nature of resonance. The current thesis focus on how this wave-function are modified.

Chapter 3

The Feshbach resonance in two-body physics

As discussed in Sec. 2.3, a two-particle interaction in a dilute system is often approximated by a pseudo-potential characterized with a s-wave scattering length a_s. The drastic change of a_s obtained by tuning the energy difference between two channels through a magnetic field in the Feshbach resonance gives experimentalists a rare ability to tune the interaction strength between two atoms. And this possibility is extremely useful to study BEC-BCS crossover where the interaction varies from weak to strong.

Here we briefly review the Feshbach resonance in a two-body system. As discussed in Chapter 2, a hyperfine level is an eigenstate for an isolated single atom. However, when two atoms interact, most of the interaction comes from electrons with only negligible effects from nucleons . As a result, hyperfine levels are no longer true eigenstates of the two-body system. Nevertheless, hyperfine levels can serve as good approximated quantum numbers and we are going to call a pair of hyperfine indices a "channel". Different channels in general have different interactions. They are decoupled at the lowest order. In a magnetic field, different channels differ in energy at threshold, where two atoms are infinitely away from each other, due to the Zeeman energy which is mostly determined by the electronic magnetic moment because the electronic magnetic moment is much larger than the nuclear magnetic moment. This energy difference is easy to tune through a magnetic field.

When the mixing between channels are taken into consideration, the simple single-channel scattering becomes the multi-channel scattering. Especially, when the one channel's threshold is close to a bound-state in the other channel, the low-energy scattering property of that channel is dramatically altered. Its phase shift changes 2π; its s-wave scattering length a_s blows to infinity and then jumps to the infinity of the opposite sign. This is essentially what happens in a Feshbach resonance, studied by Fano [Fano, 1961] and Feshbach [Feshbach, 1962] for nuclear and atomic physics in 1960s. Here we mostly follow the treatment by Leggett [Leggett, 2006] (with some different symbols to comply with the rest of this thesis). [1]

[1] In order to be consistent with other parts of the thesis, we here use some different symbols comparing to the original works by Leggett [Leggett, 2006]. Here we list them, with the symbols from [Leggett, 2006] in parenthesis. U ($= -V$): open-channel interaction; V ($= -V_c$): closed-channel interaction; Y ($=$-$g \cdot f$): inter-channel coupling; E_b ($= \epsilon_0$): binding energy of the closed-channel bound state; r_c ($= r_0$): potential range; η ($= \epsilon_0 + \tilde{\delta}$): the Zeeman energy difference between two channels; $\mathcal{K}$ ($= \kappa$) see its definition in Eq.3.12.

The Hamiltonian for the coupled open- and closed- channel can be written as a 2×2 matrix

$$\hat{H}(r) = \begin{pmatrix} -\frac{\hbar^2}{2m_r}\nabla^2 - U(r) & -Y(r) \\ -Y(r) & -\frac{\hbar^2}{2m_r}\nabla^2 + \eta - V(r) \end{pmatrix} \tag{3.1}$$

where the zero energy is taken as the energy of two atoms in the open-channel with infinite separation. η is the difference in the Zeeman energies of the two channels. The first column (row) stands for the open-channel and the second column (row) stands for the closed-channel. All the interactions are short-range. For a s-wave solution, we have the radial part as

$$\psi(r) = \frac{1}{r}\begin{pmatrix} \chi(r) \\ \chi_c(r) \end{pmatrix} \tag{3.2}$$

The coupled time-independent Schrödinger equations in the radial direction read as:

$$-\frac{\hbar^2}{2m_r}\chi'' - U\chi - Y\chi_c = E\chi \tag{3.3}$$

$$-\frac{\hbar^2}{2m_r}\chi_c'' + \eta\chi_c - V\chi_c - Y\chi = E\chi_c \tag{3.4}$$

We now expand the closed-channel component χ_c over the eigenstates of the isolated closed-channel Hamiltonian, $\chi_c = \sum_i c_i\phi_i$, where ϕ_i satisfies Schrödinger equation of the isolated closed-channel

$$-\frac{\hbar^2}{2m_r}\phi_i'' - V\phi_i = -E_b^{(i)}\phi_i \tag{3.5}$$

We denote ϕ_0 the wave function in resonance and c_0 its coefficient. Here we assume that the energy differences between eigenstates, ϕ_i's, are larger than any other energy scales in the problem. This guarantees c_0 dominates any other c_i's. So, $\chi_c \approx c_0\phi_0$. Naïvely speaking, the resonance is expected to happen at the point where the closed-channel bound state has its energy exactly at the threshold of the open-channel. This leads us to introduce the relative detuning, $\tilde{\delta} = \eta - E_b$. By comparing Eq. 3.3 and Eq. 3.5, it is easy to show

$$\chi_c = \frac{\phi_0}{E - \tilde{\delta}}\int dr'\,\phi_0^*(r')Y(r')\chi(r') \tag{3.6}$$

provided that ϕ_0 is normalized (for radial component). Inserting the expression of χ_c into the Schrödinger

equation of the open-channel component χ, Eq. 3.3, we get

$$-\frac{\hbar^2}{2m_r}\chi'' - (U+E)\chi + \frac{1}{E-\tilde{\delta}}\int_0^\infty K(r\,r')\chi(r')dr' = 0 \tag{3.7}$$

where the kernel $K(r\,r')$ is

$$K(r\,r') \equiv \phi_0(r)\phi_0(r')Y(r')Y(r) \tag{3.8}$$

The Schrödinger equation of the decoupled open-channel is

$$-\frac{\hbar^2}{2m_r}\chi'' - (U+E)\chi_0 = 0 \tag{3.9}$$

Note that $\chi_0(r) \overset{r\to 0}{\to} 0$ and $\chi_0(r) \overset{r\to\infty}{\to} A(1-r/a_{bg})$, where a_{bg} is the background s-wave scattering length of the isolated open-channel.[2] Multiply Eq. 3.7 by χ_0 and Eq. 3.9 by χ, integrate from $r=0$ to a distance r_0 much larger than the potential range, r_c, subtract them, we find,

$$\int_0^{r_0} dr\,[\chi_0(r)\chi''(r) - \chi_0''(r)\chi(r)] + \frac{2m_rE}{\hbar^2}\int_0^{r_0} dr\chi_0(r)\chi(r) = \frac{2m_r/\hbar^2}{E-\tilde{\delta}}\int_0^{r_0} dr\int_0^{r_0} dr'\chi_0(r)K(rr')\chi(r')$$

Using the Green's theorem on the first integral, we find

$$\chi_0(r_0)\chi'(r_0) - \chi_0'(r_0)\chi(r_0) + \frac{2m_rE}{\hbar^2}\int_0^{r_c} dr\chi_0(r)\chi(r) = \frac{2m_r/\hbar^2}{E-\tilde{\delta}}\int_0^{r_0} dr\int_0^{r_0} dr'\chi_0(r)K(rr')\chi(r') \tag{3.10}$$

Here we can use the boundary condition by $\chi_0(r) \overset{r\to\infty}{\to} A(1-r/a_{bg})$, $\chi(r) \overset{r\to\infty}{\to} \tilde{A}(1-r/a_s)$. $Y(r)$ is a short-range interaction and thus $K(r,r')$ only picks the short-range parts of $\chi(r)$ and $\chi_0(r)$, which varies little for different detuning. Consequently, the R.H.S approaches a constant. For the scattering solution at $E=0$, the last terml on the L.H.S. is zero, and we have

$$\frac{1}{a_s} - \frac{1}{a_{bg}} = \frac{2m_r/\hbar^2}{\tilde{\delta}}\int_0^\infty dr\int_0^\infty dr'\chi_0(r)K(rr')\chi(r') \tag{3.11}$$

Contrary to the previous guess, a_s does not diverge at the point $\tilde{\delta}=0$ because of the original interaction in the open-channel, a_{bg}. We can introduce a quantity $\mathcal{K}$, the detuning where a_s diverges, through the implicit equation ($\mathcal{K}$ shows up in R.H.S as well)

$$\mathcal{K} \equiv -\frac{2m_ra_{bg}}{\hbar^2}\int_0^\infty dr\int_0^\infty dr'\chi_0(r)K(rr')\chi_{\tilde{\delta}=\mathcal{K}}(r') \tag{3.12}$$

[2]Note that we are dealing with the internal wave function χ_0 here, i.e. the wave-function in the region $\mathcal{I}$, instead of the external wave function as in Sec. 2.3; therefore, the boundary condition for $r\to 0$ in Sec. 2.3 actually corresponds the boundary condition $r\to\infty$ here.

And if we define the "real detuning" $\delta \equiv \tilde{\delta} - \mathcal{K}$, which is the detuning from the real resonant point, where $a_s \to \pm\infty$, we have

$$a_s(\delta) = a_{bg}\left(1 + \frac{\mathcal{K}}{\delta}\right) \tag{3.13}$$

This is consistent with the empirical formula of the Feshbach resonance

$$a_s(B) = a_{bg}\left(1 + \frac{\Delta B}{B - B_0}\right) \tag{3.14}$$

where B_0 is the magnetic field at which the a_s diverges, i.e., the resonant point. Comparing the above two equations, we see that $\Delta B = \mathcal{K}(\partial\delta/\partial B)^{-1}$.

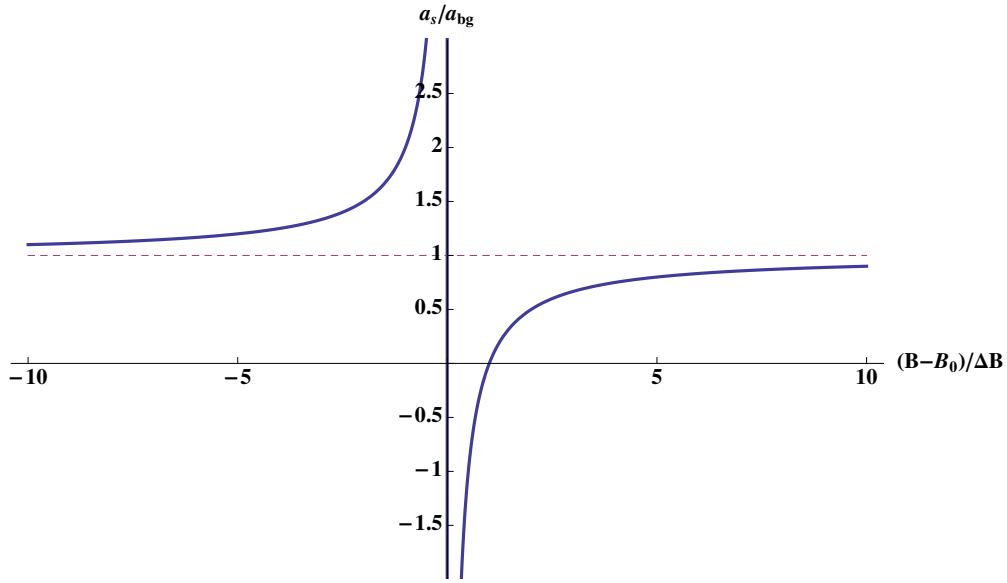


Figure 3.1: S-wave scattering length in Feshbach resonance
The dashed line is $y = a_{bg}$.

Let us now consider the bound state,[3] where $E < 0$. We define

$$a_b(E) \equiv \frac{\hbar}{(2m_r\,|E|)^{1/2}} \tag{3.15}$$

Here, we only study the bound state close to threshold with a binding energy much smaller than the binding

[3]We wish to stress again the difference between a uncoupled closed-channel bound-state ϕ_i and a real bound state formed by atoms from both open- and closed-channel. The closed-channel bound state, ϕ_i, is the eigenstate of the isolated closed-channel Hamiltonian. It is not a real eigenstate for the full two-channel Hamiltonian. On the other hand, the full Hamiltonian has bound eigenstates (i.e. $E < 0$) at large negative detuning (in the two-body context). The bound state solution for a two-channel eigenstate has components in both the open-channel and the closed-channel. The open-channel weight is often larger when close to the resonance; consequently, such bound-states are often called open-channel bound-states. Only at large negative detuning, the real two-channel bound state, mostly composed of close-channel component, coincides with the close-channel bound-state, ϕ_i to a large degree.

energy of the uncoupled closed-channel bound state, ϕ_0, namely, $|E| \ll E_b$. Therefore, we have $a_b \gg a_c$. Outside the range of potential r_c, the wave function is proportional to e^{-r/a_b}. For $r_c \ll r \ll a_b$, this wave-function can be expanded as $1 - \frac{r}{a_b}$, just as the Bethe-Peierls boundary condition (or the s-wave scattering wave function) we discussed in Chapter 2.3. Note that $a_b(E)$ is not identified as a_s a priori. Through a procedure similar as previous, it is not hard to find

$$\frac{a_{bg}}{a_b} - 1 = \frac{-\mathcal{K}}{\delta + \mathcal{K} - E} \tag{3.16}$$

We have assumed the short-range part of the bound-state wave function χ does not change much from the short-range part of the scattering state [4]; therefore $\mathcal{K}$ stays like a constant. Provided both δ and $|E|$ are much smaller than $\mathcal{K}$, this yields

$$a_b = a_{bg} \frac{\mathcal{K}}{\delta - E} \tag{3.17}$$

It is not hard to see that a_b indeed coincides with the s-wave scattering length a_s in Eq. 3.13 when $|E| \ll |\delta|$. Thus we will use a_b and a_s interchangeably hereafter. This is actually an example of our discussion about the Bethe-Peierls boundary condition in Chapter 2.3. Using the concept of the Bethe-Peierls boundary condition, we do not need to distinguish the zero energy scattering state and the negative energy bound state, and we can arrive the same conclusion easily.

Using Eqs. 3.15 and 3.17, it is easy to obtain an equation for E

$$(|E| + \delta)^2 - 2\delta_c |E| = 0 \tag{3.18}$$

where δ_c is defined as

$$\delta_c \equiv \frac{\mathcal{K}^2}{\hbar^2 / m_r a_{bg}^2} \tag{3.19}$$

And the solution for the negative detuning, i.e. $\delta < 0$, is

$$|E| = \delta_c - \delta - \sqrt{\delta_c^2 - 2\delta\delta_c} \tag{3.20}$$

We can also calculate the "relative weight" on probability of the closed-channel for a normalized open-channel

[4] This is guaranteed by the boundary condition of $\chi(r) \to 1 - r/a_s$, which fixes the normalization of the short-range part of the wave function ($\chi r \to 0$) to be the same, namely 1. As a result, all the integral term over the short-range kernel $\iint dr dr' K(r, r') \chi_0(r) \chi(r')$ give the similar value as $\mathcal{K}$ at the resonant point, Eq. 3.12.

component, χ_n, of the wave function ($\int \chi_n(r)^2 dr = 1$).[5]

$$\lambda = \left(\frac{1}{E-\tilde{\delta}}\right)^2 \left| \int dr' \phi_0(r') Y(r') \chi_n(r') \right|^2 \tag{3.21}$$

Comparing this with Eq. 3.12, and assuming the short-range part of $\chi_n(r)$ does not differ from $\chi_o(r)$ much except the normalization, we find

$$\lambda = \frac{1}{(E-\tilde{\delta})^2} \frac{\hbar^2}{2m_r a_{bg}} \frac{\mathcal{K}}{a_b} \tag{3.22}$$

For $|\delta| \lesssim \delta_c \ll \mathcal{K}$, we have

$$E - \tilde{\delta} \approx \mathcal{K} \tag{3.23}$$

We can simplify λ further

$$\lambda \approx \frac{\hbar^2}{2m_r a_{bg}} \frac{1}{(\mathcal{K} a_b)} = \left(\frac{|E|}{2\delta_c}\right)^{1/2} \tag{3.24}$$

This shows that δ_c is a "characteristic" energy scale. When $|\delta| \gg \delta_c$, Eq. 3.20 gives $E \approx \delta$, and the above equation gives $\lambda = \sqrt{|\delta|/(2\delta_c)} \gg 1$: this simply means that when the negative detuning is large, weight is predominently in the closed-channel; the real mixed bound state is a closed-channel bound state (ϕ_0) slightly dressed with the open-channel component; therefore the binding energy is very close to the binding energy of the uncoupled closed-channel bound state, ϕ_0. The often quoted relation between a_s and the binding energy, Eq. 3.15, is not valid here. On the contrary, when $|\delta| \ll \delta_c$, Eq. 3.20 gives $|E| \approx \delta^2/\delta_c \ll |\delta|$, and Eq. 3.24 then gives $\lambda \approx \delta/(\sqrt{2}\delta_c) \ll 1$. Here, the closed-channel weight is much smaller than that of the open-channel; the real bound-state is essentially an open-channel affair with little dress-up from the closed-channel. Eq. 3.15 is valid in this case.

When dealing with many-body problems, another important energy scale comes into play, namely, the Fermi energy, E_F. When E_F is much smaller than δ_c, i.e. a *broad resonance*, the closed-channel has only negligible weight close to resonance, which is the situation of interest. In such a case, it is a good approximation to take the Feshbach resonance as only a knob to tweak the interaction in the open-channel. On the contrary, when E_F is close or even larger than δ_c, i.e. a *narrow resonance*, the closed-channel weight can be significant clsoe to resonance; as a result, it is necessary to explicitly take the closed-channel into account in the many-body framework.

One important remark about the above discussion is that whether a resonance is "broad" or "narrow" is a many-body concept and is relative. For one particular resonance with a fixed δ_c, in a infinite dilute system

[5]Note here the normalization on $\chi(r)$ is different from the most cases of this section, where $\chi(r)$ is normalized by requiring $\chi \overset{r\to\infty}{\to} (1 - r/a_b)$ or e^{-r/a_b} here. The difference is an extra $(a_b)^{-1/2}$ for the wave function and that contributes the extra factor a_b^{-1} in Eq. 3.24.

(i.e. a two-body system) with a zero Fermi energy, $E_F = 0 \ll \delta_c$, it is a broad resonance. As the system becomes denser and denser, E_F increases and the resonance becomes less and less broad; finally, when E_F is in the order or even larger than δ_c, the resonance becomes a narrow one. In the real experimental system of the ultracold alkali gases, the achievable density has a certain range, so does the Fermi energy range, E_F; therefore the "broadness" or "narrowness" of a resonance is not as flexible.

Chapter 4

The single-channel BEC-BCS crossover

In this chapter, we briefly review the BEC-BCS crossover in a single channel. The idea to describe the BEC and BCS on the same footing stems back several decades [Eagles, 1969, Leggett, 1980, Nozières and Schmitt-Rink, 1985, Randeria, 1995]. The BCS theory can be understood as the following: fermions form "giant molecules" and those molecules then condense simultaneously. It is not hard to show that the BCS ansatz is equivalent to the coherent state of a two-body pair $\psi^\dagger = \sum_{\mathbf{k}} c_{\mathbf{k}} a^\dagger_{\uparrow\mathbf{k}} a^\dagger_{\downarrow-\mathbf{k}}$

$$\prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\uparrow\mathbf{k}} a^\dagger_{\downarrow-\mathbf{k}}) \left|0\right\rangle = A \exp\left(\sum_{\mathbf{k}} c_{\mathbf{k}} a^\dagger_{\uparrow\mathbf{k}} a^\dagger_{\downarrow-\mathbf{k}}\right) \left|0\right\rangle \tag{4.1}$$

where $c_{\mathbf{k}} = (v_{\mathbf{k}}/u_{\mathbf{k}})$. The size of these "giant molecules" is much larger than the interparticle distance. Moving away from the BCS end toward the BEC end, pairs shrink as the interparticle attraction becomes stronger. On the BEC side, two-fermion molecules are smaller than the interparticle distance and therefore a well-defined object. However, the binding energy now is much larger than the typical many-body energy scale and condensation does not happen at the same time when molecules form. Nevertheless, at low enough temperature, we can still consider the formation of molecules and their condensation at the same time, compatible with the the same framework used for BCS.

In the single-channel BEC-BCS crossover model, one imagines a "magic" knob that can tune the interaction strength along the crossover. The many-body fermion system sweeps from BCS of a fermionic atom system to BEC of diatomic molecules in response to the increase of attraction. This directly applies to the broad-resonance of the two-channel case as well, where the closed-channel weight is negligible and only serves to modify the effective interaction strength in the open-channel. We mostly follow the path-integral treatment by Randeria and the company [Randeria, 1995, Engelbrecht et al., 1997, Diener et al., 2008]. They have studied this problem with a path integral approach which is proved to be a nice tool for the problem due to its flexibility and readiness to be extended for the higher order fluctuations. In the next two chapters, this method will be adapted further for the two-channel model.

We start with an attractive δ-potential in the coordinate space. This potential is not equivalent to the

reduced pairing potential used in the original BCS work. The reduced pairing potential only couples particles of the opposite momentum and does not support simple form of Hubbard-Stratonovich transformation, which is essential to solve the problem in the path integral formulation.

The Hamiltonian with the chemical potential of the system can be written as

$$\hat{H} - \mu\hat{N} = \sum_{\sigma} \int d^d\mathbf{r} c_\sigma^\dagger(\mathbf{r}) \left(-\frac{1}{2m}\nabla^2 - \mu \right) c_\sigma(\mathbf{r}) - g \int d^d\mathbf{r} c_\uparrow^\dagger(\mathbf{r}) c_\downarrow^\dagger(\mathbf{r}) c_\downarrow(\mathbf{r}) c_\uparrow(\mathbf{r}) \tag{4.2}$$

Introducing the quantum partition function $\mathcal{Z} = \int \mathcal{D}(\bar{\psi}, \psi) \exp\left(-S[\bar{\psi}, \psi]\right)$, where $\mathcal{D}(\bar{\psi}, \psi)$ denotes the functional integral over all possible wave function ψ and $\bar{\psi}$, and the action $S[\bar{\psi}, \psi]$ can be written down from the Hamiltonian

$$S[\bar{\psi}, \psi] = \int_0^\beta d\tau \int d^d\mathbf{r} \left[\sum_\sigma \bar{\psi}_\sigma(\mathbf{r}, \tau) \left(\partial_\tau - \frac{1}{2m}\nabla^2 - \mu \right) \psi_\sigma(\mathbf{r}, \tau) - g\bar{\psi}_\uparrow(\mathbf{r}, \tau)\bar{\psi}_\downarrow(\mathbf{r}, \tau)\psi_\downarrow(\mathbf{r}, \tau)\psi_\uparrow(\mathbf{r}, \tau) \right] \tag{4.3}$$

The fermion fields ψ_σ and $\bar{\psi}_\sigma$ are two independent Grassmann variables. Notice that they are not complex conjugate to each other as in the usual operator language because complex conjugate is not a well-defined concept for Grassmann variables.

This system can be solved with Hubbard-Stratonovich transformation. Introduce an auxiliary field (functional variable) $\Delta(\mathbf{r}, \tau)$ coupled with a pair $\psi_\uparrow(\mathbf{r}, \tau)\psi_\downarrow(\mathbf{r}, \tau)$. We write down first the Gaussian integral of Δ

$$1 = \int \mathcal{D}(\bar{\Delta}, \Delta) \exp\left(-\frac{1}{g} \int d\tau d^d r \bar{\Delta}\Delta \right) \tag{4.4}$$

Note that we absorb the extra constant of integration into the measure of $\mathcal{D}(\bar{\Delta}, \Delta)$. And with a shift of $\Delta(\mathbf{r}, \tau) \to \Delta(\mathbf{r}, \tau) - g\psi_\uparrow(\mathbf{r}, \tau)\psi_\downarrow(\mathbf{r}, \tau))$, we have [1]

$$\exp\left(g \int d\tau d^d\mathbf{r} \bar{\psi}_\uparrow\bar{\psi}_\downarrow\psi_\downarrow\psi_\uparrow \right) = \int \mathcal{D}(\bar{\Delta}, \Delta) \exp\left\{ -\int d\tau d^d\mathbf{r} \left[\frac{1}{g}\bar{\Delta}\Delta - \left(\bar{\Delta}\psi_\downarrow\psi_\uparrow + \Delta\bar{\psi}_\uparrow\bar{\psi}_\downarrow \right) \right] \right\} \tag{4.5}$$

Note that $\Delta(\mathbf{r}, \tau)$ (or $\bar{\Delta}(\mathbf{r}, \tau)$) comes from Grassmann fields $\psi(\mathbf{r}, \tau)$ (or $\bar{\psi}(\mathbf{r}, \tau)$). Therefore, they are not related to each other as complex conjugate either. Nevertheless, at the mean field level or only at the phase fluctuation around the mean field values, Δ and $\bar{\Delta}$ are indeed complex conjugate. Consequently, we will just take Δ as normal bosonic field in the following and often simply treat $\bar{\Delta}$ as Δ's complex conjugate. Now

[1] $\int \mathcal{D}(\bar{\Delta}, \Delta) \cdot 1$ is only a constant factor on partition function $\mathcal{Z}$ and has no effect on real physical quantity; therefore, we can take it as 1. (This is equivalent to divide the $\mathcal{Z}$ by a constant)

the interaction term can be replaced.

$$\mathcal{Z} = \int \mathcal{D}(\bar{\psi},\psi) \int \mathcal{D}(\bar{\Delta},\Delta) \exp\left\{ -\int d\tau d^d\mathbf{r} \left[\sum_\sigma \bar{\psi}_\sigma \left(\partial_\tau - \frac{1}{2m}\nabla^2 - \mu \right) \psi_\sigma + \frac{1}{g}\bar{\Delta}\Delta - \left(\bar{\Delta}\psi_\downarrow\psi_\uparrow + \Delta\bar{\psi}_\uparrow\bar{\psi}_\downarrow \right) \right] \right\}$$

At the expense of introducing an auxiliary field (Δ) which has contact-type coupling to the original field ψ, we eliminate the four-field interaction term formally. Δ field is like a *local potential* for ψ, although this *local potential* has to be calculated from the original field self-consistently. Nevertheless, Δ couples to a pair of fermionic field ψ, and thus it extracts a special degree of freedom from the ψ field. When properly selected, this degree of freedom is highly non-trivial and has macroscopic importance, which serves as the "order parameter" for the system. The above formula for partition function is bilinear to ψ, and we can rewrite it into a nicer form in Nambu spinor representation

$$\bar{\Psi} = \begin{pmatrix} \bar{\psi}_\uparrow & \psi_\downarrow \end{pmatrix}, \qquad \Psi = \begin{pmatrix} \psi_\uparrow \\ \bar{\psi}_\downarrow \end{pmatrix} \tag{4.6}$$

$$\mathcal{Z} = \int \mathcal{D}(\bar{\Psi},\Psi) \int \mathcal{D}(\bar{\Delta},\Delta) \exp\left\{ -\int d\tau d^d\mathbf{r} \left[\frac{1}{g}\bar{\Delta}\Delta - \bar{\Psi}\hat{\mathcal{G}}^{-1}\Psi \right] \right\} \tag{4.7}$$

where

$$\hat{\mathcal{G}}^{-1} = \begin{pmatrix} [\hat{G}_0^{(p)}]^{-1} & \Delta \\ \bar{\Delta} & [\hat{G}_0^{(h)}]^{-1} \end{pmatrix} \tag{4.8}$$

is known as the Gor'kov Green function. $[\hat{G}_0^{(p)}]^{-1} = -\partial_\tau + \frac{1}{2m}\nabla^2 + \mu$, and $[\hat{G}_0^{(h)}]^{-1} = -\partial_\tau - \frac{1}{2m}\nabla^2 - \mu$ represent the non-interacting Green's functions of the particle and the hole respectively.

Before going further, we would like to discuss one confusing point about the possible one-or-two indices for quantities such as G or Δ in Eq. 4.8. As a matrix, such a quantity has two indices (x, x') or (p, p'), which have no ambiguity in usage. On the other hand, there are often ambiguity when only one index x or p is used. In some cases, the one index means the relative value of the two indices. For example, an interaction, $U(\mathbf{r}_1, \mathbf{r}_2)$, normally only depends on the relative coordinate, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. So $U(\mathbf{r})$ means $U(\mathbf{r}_0 + \mathbf{r}, \mathbf{r}_0)$. In other cases, especially common in the current thesis, the one index stands for its repetition. In this case, the difference is always zero. For example, the free Green's function, $G_0(p)$ stands for $G_0(p,p')\delta(p-p')$. Similarly, the order parameter, $\Delta(x)$, only couples to $\bar{\psi}(x)\bar{\psi}(x)$ (Eq. 4.5). When used in the matrix context (Eq. 4.8), it means $\Delta(x)\delta(x-x')$. Interestingly, its Fourier transformation in momentum space does not have the same properties. In fact, it means $\Delta(p,p') = \Delta(p'-p)$.

Now action in Eq. 4.7 is bilinear to Ψ; so it can be integrated out formally and the partition function then only depends on the field Δ.

$$\mathcal{Z} = \int \mathcal{D}(\bar{\Delta}, \Delta) \exp\left\{ -\left[\left(\int d\tau d^d r \frac{1}{g} \bar{\Delta}\Delta \right) - \ln\det \hat{\mathcal{G}}^{-1} \right] \right\} \tag{4.9}$$

And the action becomes

$$S[\bar{\Delta}, \Delta] = \left[\left(\int d\tau d^d r \frac{1}{g} \bar{\Delta}\Delta \right) - \ln\det \hat{\mathcal{G}}^{-1} \right] \tag{4.10}$$

Note that the determinant in $\ln\det \hat{\mathcal{G}}^{-1}$ runs through both the normal coordinate space and 2×2 Nambu spinor space. The above formulas are exactly equivalent to the original partition function (action) in the fermion field ψ (Eq. 4.3). It looks nice and compact. Nevertheless, $\ln\det \hat{\mathcal{G}}^{-1}$ term is highly non-trivial and contains all the many-body physics.

4.1 Mean field results

The saddle point equation of Eq. (4.9) gives the mean-field result of the system. First we need to find the derivative of $\ln\det \hat{\mathcal{G}}^{-1}$. We notice the identity

$$\ln\det \hat{A} = \mathrm{tr}\ln \hat{A} \tag{4.11}$$

and differential rule of the function "tr ln"

$$\frac{\delta}{\delta\phi_q} \mathrm{tr}\ln(\hat{\mathcal{G}}^{-1}) = \mathrm{tr}(\hat{\mathcal{G}} \frac{\delta}{\delta\phi_q} \hat{\mathcal{G}}^{-1}) \tag{4.12}$$

Using the above relations, we can write the saddle equation of Eq. (4.9) (differential with respect to Δ) as

$$\frac{1}{g}\bar{\Delta}(\mathbf{r}, \tau) - \mathrm{tr}\left[\hat{\mathcal{G}}(\mathbf{r}, \tau, \mathbf{r}, \tau) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right] = 0 \tag{4.13}$$

Here this matrix is in the Nambu spinor space. At the mean field level, we seek a tempo-spacial homogeneous solution of $\Delta(x) = \Delta_0$. At this level, $\Delta(p)$ becomes a δ-function in the frequency-momentum space, and has non-zero elements only for two fermions with the same momentum. (Please See the discussion in the previous section about one vs. two indices. This is not generally true in other situations, as we show it when discussing collective modes in sec. 4.2) We can find the Gor'kov Green function from Eq. (4.8) in

momentum space at the mean-field level

$$G_{0\,p,p'} = \frac{1}{(i\omega_n)^2 - E_{\mathbf{p}}^2} \begin{pmatrix} i\omega_n + \xi_{\mathbf{p}} & -\Delta_0 \\ -\bar{\Delta}_0 & i\omega_n - \xi_{\mathbf{p}} \end{pmatrix} \delta_{p=p'} \equiv G_0(p)\delta_{p=p'} \tag{4.14}$$

Here p is the frequency-momentum, $p = (\omega_n, \mathbf{p})$, and ω_n is the Matsubara frequency of Fermions. $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, $\epsilon_{\mathbf{k}} = \mathbf{k}^2/2m$, $E_{\mathbf{p}} = \sqrt{\xi_{\mathbf{p}}^2 + |\Delta_0|^2}$. And the saddle point equation can be rewritten as

$$\frac{1}{g}\bar{\Delta}_0 = \frac{T}{\mathcal{V}_0}\sum_{\mathbf{p},n} \frac{\bar{\Delta}_0}{\omega_n^2 + E_{\mathbf{p}}^2} \tag{4.15}$$

Here T is the temperature, and $\mathcal{V}_0$ is the volume in d-dimension. The summation of the Matsubara frequency can be evaluated[2] and we find

$$\frac{1}{g} = \frac{1}{\mathcal{V}_0}\sum_{\mathbf{p}} \frac{1 - 2n_f(E_p)}{2E_p} = \frac{1}{\mathcal{V}_0}\sum_{\mathbf{p}} \frac{\tanh\left(E_p/2T\right)}{2E_p} \tag{4.16}$$

where $n_f(\epsilon)$ is the fermi distribution function. This is exactly the famous gap equation obtained from other methods as well. On the other hand, $\hat{\mathcal{G}}^{-1}$ in Eq. (4.8) is the inverse of the fermion-fermion correlation of Ψ. In the mean field, G_0 as Eq. (4.14) can be diagonalized in the momentum space with a canonical (Bogoliubov) transformation. We can make an analytic continuation of $i\omega_n \to \omega + 0^+$. Eq. (4.14) then has poles ($\pm E_p$) where $\omega^2 - E_{\mathbf{p}}^2 = 0$, which determine the spectrum of fermionic excitations. Indeed, in the BCS-like states ($\mu > 0$), the spectrum is gapped at Δ; while in the BEC-like states ($\mu < 0$), the fermionic excitation starts from the molecule binding energy $\sqrt{\mu^2 + \Delta^2} \approx |\mu|$.

The summation in Eq. (4.16) does not converges in 3D because the summand does not decreases fast enough. This is because our assumption of contact interaction breaks down for the scale smaller than real potential range r_c, i.e., the summation of momentum is capped at some high momentum Λ related to $1/r_c$. Notice that in 3D, we have a similar relation that connect the bare potential g to a more physically observable quantity, the s-wave scattering length a_s

$$\frac{m\mathcal{V}_0}{4\pi a_s} = -\frac{1}{g} + \sum_{k<\Lambda} \frac{1}{2\epsilon_{\mathbf{k}}} \tag{4.17}$$

[2]The summation of the Matsubara frequency of a function $h(i\omega_n)$ is carried out by the normal trick. We multiply $h(z)$ with the Fermi distribution function $n_F(z)$, the summation is the sum of residuals at the imaginary axis of $n_F(z)$. The contour can be deform into a contour over the rest of singular points of $h(z)$. We just need to find the residuals of the total function $h(z)n_F(z)$ over those singular points to find the Matsubara summation. However, due to zero temperature, the $n_F(z)$ is only nonzero at the negative singular points of $h(z)$, $-E_{\mathbf{k}}$ in this case. (The other singular point, $E_{\mathbf{k}}$, gives $n_F(E_{\mathbf{k}}) = 0$ for zero temperature.)

Here $\mathcal{V}_0$ is the total volume. We can renormalize Eq. 4.16 with this relation

$$-\frac{m\mathcal{V}_0}{4\pi a_s} = \sum_{\mathbf{k}} \left[\frac{\tanh\left(E_k/2T\right)}{2E_k} - \frac{1}{2\epsilon_{\mathbf{k}}} \right] \tag{4.18}$$

Now the gap equation has proper decay in high momentum and no artificial cutoff is necessary. There are two unknown parameters, μ and Δ, in the equation. We need another equation in order to pin them down. To complement the gap equation, we can introduce the number equation, $N = -\partial\Omega/\partial\mu$. At the saddle point, the thermodynamic potential is $\Omega_0 = S[\Delta_0]/\beta$, and we have the number equation

$$N = -\frac{1}{\beta}\mathrm{tr}\left(G_0 \frac{\partial G_0^{-1}}{\partial \mu} \right)$$

Similarly the summation (due to the trace) over the Mastubara frequency can be evaluated and we have the number equation

$$N = \frac{1}{L^d}\sum_{\mathbf{k}} \left[1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2T}\right) \right] \tag{4.19}$$

This equation has no divergence at high momentum. The number equation and the renormalized gap equation Eq. (4.18) compose the implicit equations for two unknown parameters, gap Δ and chemical potential μ. It is not hard to find the zero temperature analytic result at both ends. At the BCS end ($1/k_F a_s \to -\infty$), we obtain $\mu \approx E_F$ and $\Delta \propto \exp(-\pi/2k_F\left|a_s\right|)$; at the BEC end ($1/k_F a_s \to +\infty$), $\mu = -\hbar^2/2ma_s^2$, i.e. half of the binding energy of a molecule, while $\Delta \propto n^{1/2}a_s^{-1/2}$ no longer has much physical significance. In the more general crossover region, these two equations can only be solved numerically. They have no singularity in the whole region, which indicates it is a crossover instead of any simple phase transition. Please see Fig. 4.1 for detail.

4.2 Gaussian fluctuation and collective modes

We can expand the partition function Eq. (4.9) around the mean-field value, $\Delta(\mathbf{r},\tau) = \Delta_0 + \theta(\mathbf{r},\tau)$. The linear order of the expansion is zero because Δ_0 is the saddle point. The next order gives us the bilinear terms on θ, i.e., correlation of bosonic fields Δ. Note that here the Hamiltonian only has a contact-type potential, therefore it cannot cover the situation of a charged system where long-range Columnb interaction cannot be neglected. We limit ourselves to the neutual case. Nevertheless, it is conceivable that a more realistic short-range potential only renormalizes some parameters in the following calculation while leaves the qualitative result unmodified.

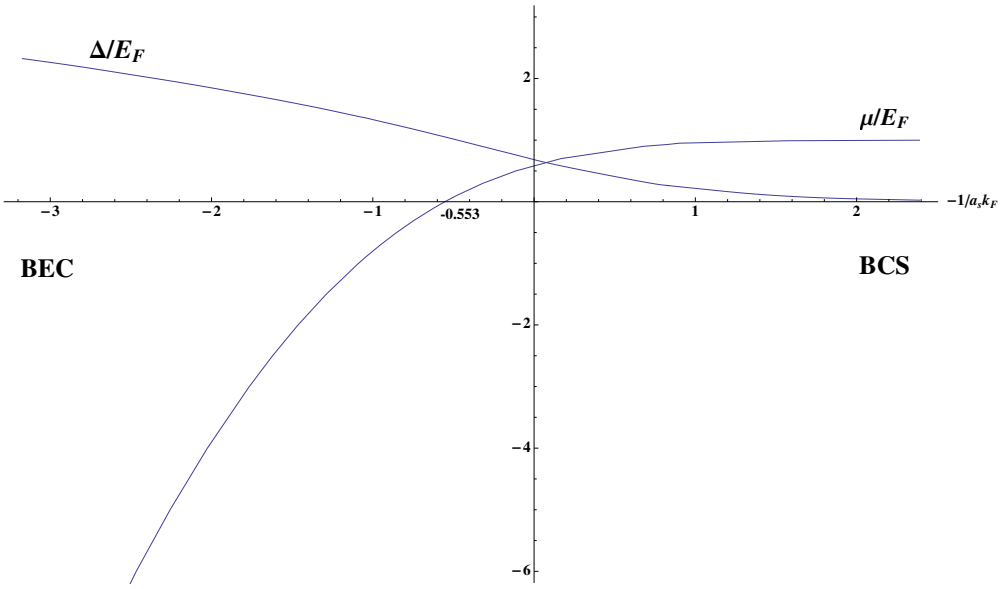


Figure 4.1: The chemical potential μ and gap Δ in the mean field level over crossover
All quantities in the unit of energy (μ, Δ) are rescaled with the Fermi energy E_F and the s-wave scattering length a_s is rescaled with $1/k_F$.

Notice that we can expand the second term in Eq. (4.9) for $\hat{G}^{-1} = \hat{G}_0^{-1} + \hat{K}$

$$\mathrm{tr}\ln\hat{G}^{-1} = \mathrm{tr}\ln{\hat{G}_0}^{-1} + \mathrm{tr}(\hat{G}_0\hat{K}) - \frac{1}{2}\mathrm{tr}(\hat{G}_0\hat{K}\hat{G}_0\hat{K}) + \cdots \tag{4.20}$$

In our case,

$$\hat{K} = \begin{pmatrix} 0 & \theta \\ \theta^* & 0 \end{pmatrix} \tag{4.21}$$

Here the linear terms of $\hat{K}$ or θ (θ^*) are zero as the saddle point condition. To the second order, the action is

$$S[\Delta_0, \theta, \theta^*] = S[\Delta_0] + \frac{1}{2g}\mathrm{tr}(\hat{K}\hat{K}) + \frac{1}{2}\mathrm{tr}(\hat{G}_0\hat{K}\hat{G}_0\hat{K}) \tag{4.22}$$

Write the last term into the momentum representation

$$\mathrm{tr}(\hat{G}_0\hat{K}\hat{G}_0\hat{K}) = \sum_{q,p} \mathrm{Tr}\left(G_0(p)K_qG_0(p-q)K_{-q}\right) \tag{4.23}$$

Notice that the second "Tr" and following "Tr" in this section only runs in Nambu spinor space and $q = (\mathbf{q}, q_l)$, $p = (\mathbf{p}, p_n)$ are all four momentum, where q_l is the bosonic Matsubara frequency while p_n is the

fermionic Matsubara frequency.

$$K_{p_0,p_0+q} = K_q = \begin{pmatrix} 0 & \theta_q \\ \theta^*_{-q} & 0 \end{pmatrix} \tag{4.24}$$

And we remember that $G_0(p) = G_{0p,p}$ If we introduce a new vector

$$\theta(q) = \begin{pmatrix} \theta_q \\ \theta^*_{-q} \end{pmatrix} \qquad \theta^\dagger(q) = \begin{pmatrix} \theta^*_q & \theta_{-q} \end{pmatrix} \tag{4.25}$$

the action can be rewritten into a more compact form

$$S[\Delta_0, \theta, \theta^*] = S[\Delta_0] + \frac{1}{2}\sum_q \left[\theta^\dagger(q)\mathbf{M}(q)\theta(q)\right] \tag{4.26}$$

Notice that we can always choose a real Δ_0 and therefore $G_{0\ 12}(p) = G_{0\ 21}(p)$, we have

$$\mathbf{M}_{q,q} = \mathbf{M}(q) = \begin{pmatrix} \frac{1}{g} + \sum_p G_{0\ 11}(p)G_{0\ 22}(p-q) & \sum_p G_{0\ 12}(p)G_{0\ 12}(p-q) \\ \sum_p G_{0\ 12}(p)G_{0\ 12}(p-q) & \frac{1}{g} + \sum_p G_{0\ 11}(p-q)G_{0\ 22}(p) \end{pmatrix} \tag{4.27}$$

The summation over the (fermionic) Matsubara frequency of p_n can be carried out at zero temperature

$$\begin{aligned} M_{11}(q) &= M_{22}(-q) \\ &= \frac{1}{g} + \sum_{\mathbf{p},p_n} G_{0\ 11}(p)G_{0\ 22}(p-q) \\ &= \frac{1}{g} + \sum_{\mathbf{p}} \left(\frac{u^2 u'^2}{iq_l - E - E'} - \frac{v^2 v'^2}{iq_l + E + E'} \right) \end{aligned} \tag{4.28}$$

$$\begin{aligned} M_{12}(q) &= M_{21}(q) \\ &= \sum_{\mathbf{p},p_n} G_{0\ 12}(p)G_{0\ 12}(p-q) \\ &= \sum_{\mathbf{p}} uvu'v' \left(\frac{1}{iq_l + E + E'} - \frac{1}{iq_l - E - E'} \right) \end{aligned} \tag{4.29}$$

where $u = u_{\mathbf{p}}$, $v = v_{\mathbf{p}}$, $E = E_{\mathbf{p}}$ and $u' = u_{\mathbf{p-q}}$, $v' = v_{\mathbf{k-q}}$, $E' = E_{\mathbf{k-q}}$. $u_{\mathbf{k}}$, $v_{\mathbf{k}}$, $E_{\mathbf{k}}$ are defined as usual BCS literature.

$$v^2_{\mathbf{k}} = 1 - u^2_{\mathbf{k}} = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \tag{4.30}$$

The $G^{(M)} = \mathbf{M}^{-1}$ is the correlation function of θ (or Δ) and its poles give the spectrum of collective modes

as every θ_q (or Δ_q) involves many fermions moving in a coherent manner. So the spectrum of collective modes can be determined by finding poles of $G^{(M)}$, $\det M(\omega, \mathbf{q}) = 0$, after we analytically continue for the frequency $iq_l \to \omega + i0^+$.

For low energy modes, where ω, $|\mathbf{q}|^2$ both are much smaller than $\min\{E_\mathbf{k}\} = \Delta_0$ (or $\sqrt{\mu^2 + \Delta^2}$ for $\mu < 0$), we can expand M with ω and $\mathbf{q}$. The lowest order has the form $\omega \approx c\,q$, which suggests a sound wave as expected for any Goldstone mode. At BCS side, $c = v_F/\sqrt{3}$, where v_F is the Fermi velocity. This coincides with the famous Anderson-Bogoliubov mode. At the BEC side, we get $c^2 = \Delta^2/8m|\mu| = v_F^2(k_F a_s)/3\pi = 4\pi n_B a_B/m_B$, which fits the low momentum part of Bogoliubov spectrum of bosons gas. Here $m_B = 2m$ is the molecule mass, $n_B = n/2$ is the molecule density and $a_B = 2a_s$ is the inferred interaction between molecules. This value differs from the result of more accurate calculation from the few-body theory, $a_B = 0.6a_s$ [Petrov et al., 2004], which indicates the possible deficiency of the current theory.

4.3 An alternative method to invert the Green's function

In the above section, we inverted the Gor'kov green function matrix Eqs. (4.8, 4.14) directly and it is not hard to do as a 2×2 matrix in the momentum space. Alternatively, we can use a different approach which proves to be more convenient in the two-channel problem. First, we diagonalize $\hat{\mathcal{G}}^{-1}$ with a unitary transformation T, in the momentum space

$$\hat{\mathcal{G}}^{-1} = \begin{pmatrix} i\omega_n - \xi_k & \Delta \\ \bar{\Delta} & i\omega_n + \xi_k \end{pmatrix} = T^\dagger B T \tag{4.31}$$

It is easy to show that such T and B satisfying above equation are

$$T = \begin{pmatrix} u_k & v_k \\ -v_k^* & u_k \end{pmatrix} \qquad B = \begin{pmatrix} i\omega_n + E_k & 0 \\ 0 & i\omega_n - E_k \end{pmatrix} \tag{4.32}$$

where $u_k^2(v_k^2) = \frac{1}{2}(1 \pm \xi_k/E_k)$ and $E_k = \sqrt{\xi_\mathbf{k}^2 + \Delta^2}$ are conventionally defined quantities in the BCS theory. Actually, this transformation is nothing but the Bogoliubov canonical transformation, and the B matrix simply describes the spectrum of the fermionic quasi-particles. Now it is easy to invert $\hat{\mathcal{G}}^{-1}$

$$\mathcal{G} = T^\dagger B^{-1} T \tag{4.33}$$

Green's function $\mathcal{G}$ takes a more conventional form $A/(i\omega_n \pm E_k)$ here without any dependency on frequency in nominator as Eq. (4.14). Matsubara frequency summation over $G_0(k)$ in the mean-field and $G_0(k)G_0(k+q)$ in the Gaussian order are then easier to perform as in text-book.

Chapter 5

The two-channel three-species many-body model, the mean field

For the narrow Feshbach resonance, atoms have considerable weight in the closed-channel and the Pauli exclusion between two channels cannot be neglected. A many-body framework needs to include both channels. Before diving into the detailed calculation, let us make some rough estimates about scales in order to build some intuition. The same problem at the two-body level is well understood as briefed in Chapter 3. We estimate how much each channel would change in a many-body system. Compared to a two-body system, the two-body correlation of a (cold) many-body fermion system in the momentum representation is modified mostly in low momentum, i.e. around or below the Fermi momentum, while staying just like the two-body wave-function intact in high momentum. The open-channel component of the two-body scattering wave-function is like a zero-energy free wave ($k = 0$) plus a small short-range kernel of size r_c. In the momentum space, this wave function is like a δ-function at $k = 0$ with a small tail in high momentum. The occupation number in the first available level, $k = 0$, is close to one (for two hyperfine spins) and this level cannot accommodate one more pair. The next pair has to occupy the next available level in k instead of the lowest energy two-body level, $k = 0$. This suggests that the open-channel requires a full many-body treatment. The situation is quite different in the closed-channel. One crucial assumption is that the closed-channel bound state is much smaller than the interparticle distance in the real representation. A closed-channel bound state, ϕ_0, in the momentum, spreads its most weight in the range $[0, 1/a_c]$. The weight in each momentum level is so tiny that it is even smaller than 1 when it is multiplied by total atoms number N, $N\left|\phi_k\right|^2 \ll 1$. It only has a very small fraction of its weight within the Fermi energy range ($< k_F$). Hence, the closed-channel only has a small overlap with atoms in the open-channel, as well as with other atoms in the closed-channel. The smallness of this overlap ensures that many-body effects in the closed-channel can be treated perturbatively. As discussed in Sec. 2.3 and Appendix B.3, the high momentum part of the two-body correlation just follows the two-body wave function; therefore, we can write two-body correlation as

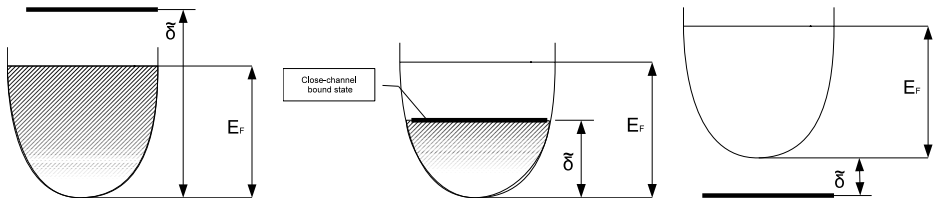
$$h_{\mathbf{k}} \sim \phi_{0\mathbf{k}} f(\mathbf{k}) \tag{5.1}$$

with $f(\mathbf{k}) = 1$ for $k \gg k_F$. $f(\mathbf{k})$ deviates from 1 in low energy and represents all the many-body correction.

In addition to the two channel description, the model needs to be explicitly expressed with the three hyperfine species at least in some part in order to address the inter-channel Pauli exclusion between two channels due to the common species. This effect has received little attention in theoretical research and a model as such is a useful addition to our knowledge of the BEC-BCS crossover and the Feshbach resonance. Nevertheless, as we just discussed, and will illustrate more quantitatively later, the effects of the inter-channel Pauli exclusion between the two channels is relatively minor and can be treated perturbatively. Consequently, it is not necessarily to carry the three species description all through the calculation. The description of two channels and the description of three species are used in different phases of the calculation to solve the problem.

5.1 The extremely narrow resonance

Before the quantitative model, we discuss qualitatively a simple yet revealing case, the extremely narrow resonance, where the inter-channel coupling approaches zero, $Y \to 0$. In this case, two channels are almost independent to each other except sharing the same chemical potentials. From the two-body discussion in Chapter 3 (Eqs. 3.8, 3.12, 3.19), the characteristic width of the resonance δ_c is zero in this case, which indicates that the resonance is always narrow no matter how dilute the system is.



(a) $E_F < \tilde{\delta}$ (b) $0 < \tilde{\delta} < E_F$ (c) $\tilde{\delta} < 0$

Figure 5.1: Extremely narrow resonance
The shaded area is occupied by atoms.

Here we assume that the atoms in the open-channel maintains a relatively clear Fermi surface, like the Fermi liquid or the BCS. The many body situation is quite straightforward. In general, three different situations exist, as Figs. 5.1a, 5.1b and 5.1c. When the closed-channel bound state level is above the Fermi sea ($E_F < \tilde{\delta}$, Fig. 5.1a), all atoms are in the open-channel and no atoms are in the closed-channel. Therefore, it is a genuine single-channel problem (only open-channel) with the original bare open-channel interaction. There is no need to considering the inter-channel Pauli exclusion. When the closed-channel bound state level is below the Fermi sea ($\tilde{\delta} < 0$, Fig. 5.1c), all atoms are in the closed-channel and no atoms are in

the open-channel. It is a simple di-atom molecule gas. There is no need to consider the inter-channel Pauli exclusion either. The interesting situation is when the closed-channel bound state level is in the Fermi sea ($0 < \tilde{\delta} < E_F$, Fig. 5.1b). The Fermi sea is then filled from the bottom (zero energy) all the way to the closed-channel bound state level in the open-channel. Then all the rest atoms go into the closed-channel. We do need to consider the inter-channel Pauli exclusion because atoms exist in both channel.

We can imagine the two channels are decoupled and each has $N^{(o)}$ ($N^{(c)}$ atoms. It is not hard to find the wave function in each case. The inter-channel Pauli-exclusion effect should be in the order of the overlap of these two wave functions. In the open-channel, the momentum space is filled with occupation 1 from the bottom up to the chemical potential μ (or $\tilde{\delta}$). In the closed-channel, as we discussed in the introduction, the occupation is roughly $1/E_b$ at the low momentum ($\lesssim E_F$), where E_b is the binding energy of the closed-channel bound state. So this effect should be roughly equal E_F/E_b.

5.2 Model set-up and the Hubbard-Stratonovich transformation

One way to approach this problem is to extend BCS ansatz and then find the set of parameters that optimizes the free energy. We can write down a three species BCS ansatz as

$$|\Psi\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} + w_{\mathbf{k}} a^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}} \right) |0\rangle \tag{5.2}$$

with normalization, $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 + |w_{\mathbf{k}}|^2 = 1$. Here "$a$" is the common species of two channels. (a, b) is the open channel and (a, c) is the closed channel. $|0\rangle$ is the vacuum state of fermions. This ansatz can be derived from a many-body coherent state of the two-body state as we did in the single-channel (Eq. 4.1),

$$|\Psi\rangle \propto \exp\left[\sum_{\mathbf{k}} (\phi^{(ab)}_{\mathbf{k}} a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} + \phi^{(ac)}_{\mathbf{k}} a^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}}) \right] |0\rangle \tag{5.3}$$

$\phi^{(ab)}$ and $\phi^{(ac)}$ are related to $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ and $w_{\mathbf{k}}$ as

$$\phi^{(ab)}_{\mathbf{k}} = \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} \tag{5.4}$$

$$\phi^{(ac)}_{\mathbf{k}} = \frac{w_{\mathbf{k}}}{u_{\mathbf{k}}} \tag{5.5}$$

We can then proceed to find the set of $(u_{\mathbf{k}}, v_{\mathbf{k}}, w_{\mathbf{k}})$ that optimizes the free energy. This method offers good intuition of the state with an explicit connection to two-body wave functions, $\phi^{(ab)}$ and $\phi^{(ac)}$, . However, it is not easy to find these parameters from optimization process. Furthermore, it is hard to extend this method

beyond the mean-field to study phenomena such as collective modes. We briefly discuss this approach in Appendix A. Instead, in this chapter, we use the path integral method, which turns out to be more convenient for this problem. The Hubbard-Stratonovich transformation provides a powerful tool for studying non-trivial degrees of freedom (order parameters) in the system. It is more or less equivalent to other approaches at the mean-filed level. But it has great advantage to be easily extended to explore the fluctuation over the mean-field result.

For a two-channel problem, we write down the Hamiltonian [1] as

$$\begin{aligned} H-\mu N=\int d^dr\Big\{ & \sum_{j=(a,b,c)}\bar{\psi}_j\left[\frac{1}{2m}(-i\nabla)^2-\mu+\eta_j\right]\psi_j \\ & -U\bar{\psi}_a(r)\bar{\psi}_b(r)\psi_b(r)\psi_a(r)-V\bar{\psi}_a(r)\bar{\psi}_c(r)\psi_c(r)\psi_a(r) \\ & -\left[Y\bar{\psi}_a(r)\bar{\psi}_b(r)\psi_c(r)\psi_a(r)+h.c.\right]\Big\} \end{aligned} \tag{5.6}$$

Here η_j is the Zeeman energy of the specific hyperfine species. a, b, c stands for the three hyperfine species defined as same as in the ansatz approach (Eq. 5.2). All the interactions (U, V, Y), are contact type, this simplifies the Hubbard-Stratonovich transformation considerably. It is plausible as we only study low-energy phenomena for the short-range potential.

A contact interaction is flat in momentum space. In other words, it pairs not only zero center-of-mass momentum pairs, but also finite center-of-mass momentum pairs. This is different from the paring interaction used in the original BCS work [Bardeen et al., 1957], which only pairs zero center-of-mass momentum, i.e. opposite-momentum, pairs. Nevertheless, the saddle point (mean-field) solution settles at the zero center-of-mass momentum pairing; therefore the mean-field solution coincides with that of variation method derived from pairing only opposite momentum atoms. On the other hand, the collective mode (fluctuation of order parameters) emerges naturally from the included non-zero center-of-mass momentum interaction. We do not need to introduce more general interaction terms beyond the simple opposite momentum pairing (e.g. the Coulomb interaction in [Anderson, 1958]) to study collective modes.

Three different types of Hilbert spaces are used in this chapter. The first one is the (infinite dimension) coordinate space and its reciprocal momentum space. The second one is the (3 dimension) space of hyperfine spin, a, b, c. These two are atom-based. The full many-body Hilbert space is N-power (also direct-product type) of the direct product of these two. As discussed previously, in some cases, instead of a 3-dimension hyperfine spin space, we use the third type of spaces, open- and closed-channel, (a, b), (a, c) (2 dimension). Strictly speaking, this one is just a subspace of the direct product of a pair hyperfine spin spaces. Neverthe-

[1] Here and hereafter in the chapter, we take $\hbar = 1$.

less, it is sufficient within our model because only these two combinations (channels) of a pair are considered. In principle, fermion fields ψ and $\bar{\psi}$ (and Δ and $\bar{\Delta}$ defined according to ψ and $\bar{\psi}$), both Grassmann numbers, are independent to each other and not related as complex conjugate[2]. This is marked by using "‾"(bar) instead of the normally used "†"(dagger) sign. In this chapter, a 3×3 matrix always refer to hyperfine spins; while a 2×2 matrix always refers to open- and closed-channel. And † sign is reserved only for hermitian conjugate of these two types of matrices.

Introduce two channels into the vector form. $(\psi\psi)$ is a column vector and $(\bar{\psi}\bar{\psi})$ is a row vector.

$$(\bar{\psi}\bar{\psi}) = \begin{pmatrix} \bar{\psi}_a\bar{\psi}_b & \bar{\psi}_a\bar{\psi}_c \end{pmatrix} \qquad (\psi\psi) = \begin{pmatrix} \psi_b\psi_a \\ \psi_c\psi_a \end{pmatrix}$$

The two-body interaction can then be written as a (2×2) hermitian matrix $\tilde{U}$ in the channel space

$$\tilde{U} \equiv \begin{pmatrix} U & Y \\ Y^* & V \end{pmatrix} \tag{5.7}$$

We can now write the Hamiltonian in a more compact form

$$H = \int d^dr \Big\{ \sum_{j=a,b,c} \bar{\psi}_j \left[\frac{1}{2m}(-i\nabla)^2 - \mu + \eta_j \right] \psi_j - (\bar{\psi}\bar{\psi})\tilde{U}(\psi\psi) \tag{5.8}$$

The finite-temperature action is

$$S(\bar{\psi},\psi) = \int_0^\beta d\tau \int d^dr \left[\sum_j \bar{\psi}_j(\partial_\tau - \frac{1}{2m}\nabla^2 - \mu + \eta_j)\psi_j - (\bar{\psi}\bar{\psi})\tilde{U}(\psi\psi) \right] \tag{5.9}$$

Similar as in Chapter 4, we can perform the Hubbard-Stratonovich transformation here. Introduce auxiliary fields (functional variables), (Δ_1, Δ_2), as a 2-component vector and start from the "fat identity", where all the integral constant is absorbed into the measure of functional integral of $\mathcal{D}(\Delta,\bar{\Delta})$ [Altland and Simons, 2010].

$$1 = \int \mathcal{D}(\Delta,\bar{\Delta}) \exp(-\int dx \Delta^\dagger \tilde{U}^{-1}\Delta) \tag{5.10}$$

$$\Delta^\dagger = (\bar{\Delta}_1, \bar{\Delta}_2) \qquad \Delta = \begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix}$$

here x is four-coordinate, $(\mathbf{r},\tau)$, $\int dx = \int_0^\beta d\tau \int d^d\mathbf{r}$.

[2]Complex conjugate is not a well-defined concept for Grassmann algebra

We can make a shift in Δ

$$\Delta \longrightarrow \Delta - \tilde{U}(\psi\psi) \tag{5.11}$$

Write it explicitly into the matrix form

$$\begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} \longrightarrow \begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} - \begin{pmatrix} U & Y \\ Y^* & V \end{pmatrix} \begin{pmatrix} \psi_b\psi_a \\ \psi_c\psi_a \end{pmatrix}$$

$$\left(\bar{\Delta}_1, \bar{\Delta}_2\right) \longrightarrow \left(\bar{\Delta}_1, \bar{\Delta}_2\right) - \begin{pmatrix} \bar{\psi}_a\bar{\psi}_b & \bar{\psi}_a\bar{\psi}_c \end{pmatrix} \begin{pmatrix} U & Y^* \\ Y & V \end{pmatrix}$$

First of all, notice that the new auxiliary field Δ is related to the mixture of two channels by a 2×2 matrix $\tilde{U}$. Also note that $\bar{\Delta}_i$ is not the complex conjugate of Δ_i in general as they are related to Grassmann fields $\psi\psi$ and $\bar{\psi}\bar{\psi}$ which are not complex conjugate to each other. But it can be verified later that, to the mean-field (saddle point) level as well as to the simple (phase-fluctuation) Gaussian level about collective modes, $\bar{\Delta}_i$ and Δ_i are indeed complex conjugate (and real for saddle point). Hence, for the simplicity, we will treat them as such hereinafter and use $\bar{\Delta}$ and Δ^* more or less arbitrarily. The other point to notice is that, $\Delta(\mathbf{r}, \tau)$ carries the the same coordinates as $\psi(\mathbf{r}, \tau)\psi(\mathbf{r}, \tau)$ (or frequency-momentum coordinates in the reciprocal space) because there is only the contact interaction. Now the "fat identity" Eq. 5.10 becomes

$$1 = \int \mathcal{D}(\Delta_j, \bar{\Delta}_j) \exp\left\{ - \int dx [\Delta^\dagger \tilde{U}^{-1} \Delta - (\bar{\psi}\bar{\psi})\Delta - \bar{\Delta}(\psi\psi) + (\bar{\psi}\bar{\psi})\tilde{U}(\psi\psi)] \right\} \tag{5.12}$$

The above equation use the fact $\tilde{U}$ is hermitian, so $\tilde{U}^\dagger \tilde{U}^{-1} = \tilde{U}^{-1}\tilde{U} = I$. It can be rearranged as

$$\exp[\int dx (\bar{\psi}\bar{\psi})\tilde{U}(\psi\psi)] = \int \mathcal{D}(\Delta, \bar{\Delta}) \exp\left\{ - \int dx [\Delta^\dagger \tilde{U}^{-1} \Delta - (\bar{\psi}\bar{\psi})\Delta - \bar{\Delta}(\psi\psi)] \right\} \tag{5.13}$$

This is now ready to be applied to the original action in Eq. 5.9,

$$S_\tau(\bar{\Delta}, \Delta, \bar{\psi}_i, \psi_i) = \int_0^\beta d\tau \int d^d r \left\{ \sum_j \bar{\psi}_j (\partial_\tau - \frac{1}{2m}\nabla^2 - \mu + \eta_j)\psi_j + [\Delta^\dagger \tilde{U}^{-1} \Delta - (\bar{\psi}\bar{\psi})\Delta - \bar{\Delta}(\psi\psi)] \right\} \tag{5.14}$$

We can introduce a spinor similar to the Nambu spinor representation in the single-channel superconductivity.

$$\bar{\Psi} = \begin{pmatrix} \bar{\psi}_a & \psi_b & \psi_c \end{pmatrix} \qquad \Psi = \begin{pmatrix} \psi_a \\ \bar{\psi}_b \\ \bar{\psi}_c \end{pmatrix} \tag{5.15}$$

The action can then be rewritten in a more compact form with respect to Ψ and $\bar{\Psi}$

$$S(\bar{\Delta}, \Delta, \bar{\psi}_i, \psi_i) = \int_0^\beta d\tau \int d^d r \left[\Delta^\dagger \tilde{U}^{-1} \Delta - \bar{\Psi} \mathcal{G}^{-1} \Psi \right] \tag{5.16}$$

where

$$\mathcal{G}^{-1} = \begin{pmatrix} -\partial_\tau + \frac{1}{2m}\nabla^2 + \mu - \eta_a & \Delta_1 & \Delta_2 \\ \bar{\Delta}_1 & -\partial_\tau - \frac{1}{2m}\nabla^2 - \mu + \eta_b & 0 \\ \bar{\Delta}_2 & 0 & -\partial_\tau - \frac{1}{2m}\nabla^2 - \mu + \eta_c \end{pmatrix} \tag{5.17}$$

Rewriting $\hat{\mathcal{G}}^{-1}$ in the frequency-momentum space, we find $\hat{\mathcal{G}}^{-1}$ decoupled in frequency and momentum.

$$\mathcal{G}^{-1} = \begin{pmatrix} i\omega_n - \xi_k - \eta_a & \Delta_1 & \Delta_2 \\ \bar{\Delta}_1 & i\omega_n + \xi_k + \eta_b & 0 \\ \bar{\Delta}_2 & 0 & i\omega_n + \xi_k + \eta_c \end{pmatrix} \tag{5.18}$$

here[3] $\xi_k = \frac{1}{2m}k^2 - \mu$. The diagonal elements of the second column/row (b) and the third column/row (c) corresponding to negative energy, because of the particular opposite choice in the spinor ($\bar{\Psi}_2\Psi_2 = \psi_b\bar{\psi}_b$ and $\bar{\Psi}_3\Psi_3 = \psi_c\bar{\psi}_c$). The non-diagonal elements mix ψ_a with $\bar{\psi}_{b,c}$ and therefore lead to a number-non-conserved theory.

If we in addition assume $\eta_a = \eta_b = 0$, $\eta_c = \eta$ (i.e., use η as the absolute Zeeman energy difference of two channels) , in frequency-momentum space,

$$\mathcal{G}^{-1} = i\omega_n I - \begin{pmatrix} \xi_k & -\Delta_1 & -\Delta_2 \\ -\bar{\Delta}_1 & -\xi_k & 0 \\ -\bar{\Delta}_2 & 0 & -(\xi_k + \eta) \end{pmatrix} \tag{5.19}$$

[3]In principle, there are two chemical potentials, μ_a and $\mu_{b,c}$ because a does not convert to b or c. But we omit this for simplicity and absorb all the difference into η_i.

The action in Eq. 5.16 is bilinear to Ψ and we can integrate out Ψ ($\bar{\Psi}$) formally

$$S(\bar{\Delta},\Delta)=\int dx\left(\bar{\Delta}\tilde{U}^{-1}\Delta-\mathrm{tr}\ln\hat{\mathcal{G}}^{-1}\right) \tag{5.20}$$

Note that at this stage $\Delta(\mathbf{r},\tau)$ is not necessarily homogeneous in space or pseudo-time as in the mean-field result.

5.3 Diagonalization of the Green's function

Eq. (5.20) looks fairly simple and compact. Nevertheless, it has all the physics in it and is not as simple as it looks. The major problem comes from the term $\mathrm{tr}\ln\hat{\mathcal{G}}^{-1}$, which includes logarithm and trace over an infinite-dimension matrix. All these operations are fairly straight-forward if we can diagonalize the Green's function (or its inverse) in a proper basis. It is not hard to see $\hat{\mathcal{G}}^{-1}$ is already decoupled in the frequency-momentum space (Eqs. 5.18, 5.19). It is however mixed in the 3×3 hyperfine-spin space. The rest of this section is dedicated to diagonalize this 3×3 matrix in the hyperfine-species space. Note that in principle, the following discussion is not limited for constant Δ, but also applies to inhomogeneous $\Delta(\omega_n,\mathbf{k})$ as well because the 3×3 hyperfine space is independent to the frequency-momentum space. Here we use the approach in Sec. 4.3 to diagonalize it. In current problem, we need to diagonalize a 3×3 matrix (Eq. 5.19), in other words, we need to figure out the Bogoliubov canonical transformation over which the Hamiltonian/action is diagonalized. Eigen-problem of the 3×3 matrix involves solving a cubic equation. An exact solution exists in principle. However, it offers little intuition to write down the exact result. Instead, the spectrum from the broad-resonance, where the only effect of the closed-channel is to modify the effective interaction of the open-channel, serves a reasonable lowest order approximation. We proceed to find the next order of correction over it (See Appendix B.1 and B.5).

We can break down the unitary transformation into two steps T and L.

$$B_{\omega_n,\mathbf{k}}=L_k^\dagger T_k^\dagger G^{-1}_{\omega_n,\mathbf{k}}T_kL_k \tag{5.21}$$

Here B_k is the diagonal matrix; T and L are both unitary transformation. We take T as the canonical

transformation at the broad resonance, i.e., when we can ignore the inter-channel Pauli exclusion.

$$T_k = \begin{pmatrix} u_k & v_k & 0 \\ -v_k & u_k & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{5.22}$$

where u_k and v_k are defined in a similar fashion as in the single-channel BCS problem

$$v_{\mathbf{k}}^2 \equiv 1 - u_{\mathbf{k}}^2 \equiv \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \tag{5.23}$$

$$E_{\mathbf{k}} \equiv (\xi_{\mathbf{k}}^2 + \Delta_1^2)^{1/2} \tag{5.24}$$

Note that here $v_{\mathbf{k}}^2$ does not carry the physical meaning of the occupation number of the (open-channel) atoms, and $E_{\mathbf{k}}$ does not stand for fermionic excitation spectrum as in Chapter 4 or Appendix A. They carry such meaning only at the broad resonance. In the narrow resonance, as we currently discuss, they are the zeroth order approximates of such quantities.

In the broad resonance, the closed-channel can be integrated out at the two-body level and only the BCS pairing in the open channel needs to be considered at the many-body level. Matrix T, however, is enough to diagonalize G^{-1} and L is simply an identity matrix. In the narrow resonance, T cannot diagonalize G^{-1} because of the inter-channel Pauli exclusion between channels. Consequently, L stands the extra correction due to Pauli exclusion in the canonical transformation. Apply T onto G^{-1}, we have

$$T_k^\dagger G^{-1}_{\omega_n,\mathbf{k}} T_k = i\omega_n I + \begin{pmatrix} -E_k & 0 & u_k\Delta_2 \\ 0 & +E_k & v_k\Delta_2 \\ u_k\Delta_2 & v_k\Delta_2 & +\xi_k + \eta \end{pmatrix} \tag{5.25}$$

We regard the off-diagonal elements as perturbation because we only seek the solution around the BCS wave function (T transform). Introduce a dimensionless scale ζ,

$$\boxed{\zeta = \frac{\Delta_2^2}{\Delta_1 \eta}} \tag{5.26}$$

Here both Δ_1 and Δ_2 are their mean-field (saddle point) values. It can be verified that $\zeta \ll 1$ (See Appendix B.5). This matrix can then be diagonalized with the unitary transformation $L_{\mathbf{k}}$ within the first order of ζ

(see Appendix B.1 for details of calculation.)

$$B_{\omega_n,\mathbf{k}} = i\omega_n I - \begin{pmatrix} E_{1\mathbf{k}} & 0 & 0 \\ 0 & -E_{2\mathbf{k}} & 0 \\ 0 & 0 & -E_{3\mathbf{k}} \end{pmatrix} \tag{5.27}$$

The dispersion spectrum of fermions is

$$E_{1\mathbf{k}} \equiv E_{\mathbf{k}} + \gamma_{1\mathbf{k}} \approx E_{\mathbf{k}} + \frac{\Delta_2^2 u_{\mathbf{k}}^2}{\xi_{\mathbf{k}} + \eta} \approx E_{\mathbf{k}} + u_{\mathbf{k}}^2 \zeta \frac{\eta}{\xi_{\mathbf{k}} + \eta} \Delta_1 \approx E_{\mathbf{k}} + u_{\mathbf{k}}^2 \Delta_1 \zeta \tag{5.28}$$

$$E_{2\mathbf{k}} \equiv E_{\mathbf{k}} + \gamma_{2\mathbf{k}} \approx E_{\mathbf{k}} - \frac{\Delta_2^2 v_{\mathbf{k}}^2}{\xi_{\mathbf{k}} + \eta} \approx E_{\mathbf{k}} - v_{\mathbf{k}}^2 \zeta \frac{\eta}{\xi_{\mathbf{k}} + \eta} \Delta_1 \approx E_{\mathbf{k}} - v_{\mathbf{k}}^2 \Delta_1 \zeta \tag{5.29}$$

$$E_{3\mathbf{k}} \equiv \xi_{\mathbf{k}} + \eta + \gamma_{3\mathbf{k}} \approx \xi_{\mathbf{k}} + \eta - \frac{\Delta_2^2}{2(\xi_{\mathbf{k}} + \eta)} \approx \epsilon_{\mathbf{k}} + \eta - \frac{\zeta}{2} \frac{\eta}{\xi_{\mathbf{k}} + \eta} \Delta_1 \approx \epsilon_{\mathbf{k}} + \eta - \frac{\zeta}{2} \Delta_1 \tag{5.30}$$

The last step of each equations is valid only for low momentum ($\sim k_F$) where $\eta \gg \xi_{\mathbf{k}}$. Here we choose the sign convention to make $E_{1,2,3}$ positive in their zeroth order. Similarly as in Eq. 5.18, the second and third diagonal elements are negative because in the spinor representation, we choose $\bar{\psi}_b$ and $\bar{\psi}_c$ for Ψ, which gives extra negative signs for quantity such as $\bar{\Psi}\Psi$ in Eq. 5.16.[4] These negative signs disappear when we restore them to the normal order $\bar{\psi}\psi$ in Sec. 6.1.

One interesting feature of this solution is that the corrections do not disappear for zero inter-channel coupling, $Y = 0$, which we discussed qualitatively in Sec. 5.1. This is because the corrections are due to the inter-channel Pauli exclusion between two channels, which continues to exist even when there is no inter-channel coupling. In fact, the inter-channel coupling, Y, contributing mostly energetically, modifies the effective interaction in the open-channel and affect the open-channel order parameters, Δ_1, greatly. By taking the broad resonance result as the zeroth order, we have taken effects of Y into consideration. On the other hand, the inter-channel Pauli exclusion or statistics is left out as the higher order correction as illustrated above. Furthermore, from Appendix B.5 (Eq. B.28), we know $\zeta \sim \frac{k_F}{\kappa}$, it is just the square root of our estimate E_F/E_b ($E_b = \hbar^2\kappa^2/2m$) in Sec. 5.1.

The extra factor of unitary transformation is

$$L_{\mathbf{k}} \approx I + \begin{pmatrix} 0 & -\frac{\Delta_1\Delta_2}{4E_{\mathbf{k}}^2} & u_{\mathbf{k}} \\ \frac{\Delta_1\Delta_2}{4E_{\mathbf{k}}^2} & 0 & v_{\mathbf{k}} \\ -u_{\mathbf{k}} & -v_{\mathbf{k}} & 0 \end{pmatrix} \frac{\Delta_2}{\eta} \equiv I + \delta_k \qquad L_{\mathbf{k}}^\dagger = I - \delta_{\mathbf{k}} \tag{5.31}$$

[4]Recall that ψ_i and $\bar{\psi}_i$ are Grassmann fields; thereore $\psi_i\bar{\psi}_i = -\bar{\psi}_i\psi_i$.

Here we use $u_{\mathbf{k}}v_{\mathbf{k}} = \Delta_1/2E_{\mathbf{k}}$. Note that L and $L^\dagger$ are unitary only to the first order of Δ_i/η. Now it is easy to express the Green's function as

$$G_{\omega_n,\mathbf{k}} = T_{\mathbf{k}} L_{\mathbf{k}} B^{-1}_{\omega_n,\mathbf{k}} L^\dagger_{\mathbf{k}} T^\dagger_{\mathbf{k}} \tag{5.32}$$

This is ready to be expanded over the perturbation in order of ζ or Δ_i/η. It is easy to see that all ω_n dependence concentrates on $B_{\omega_n,\mathbf{k}}$, which is linear in ω_n and simplifies the Matsubara frequency summation considerably.

$$G_{\omega_n,\mathbf{k}} \approx T_{\mathbf{k}} B^{-1}_{\omega_n,\mathbf{k}} T^\dagger_{\mathbf{k}} + T_{\mathbf{k}}\delta_{\mathbf{k}} B^{-1}_{\omega_n,\mathbf{k}} T^\dagger_{\mathbf{k}} - T_{\mathbf{k}} B^{-1}_{\omega_n,\mathbf{k}}\delta_{\mathbf{k}} T^\dagger_{\mathbf{k}} \equiv G^{(0)}_{\omega_n,\mathbf{k}} + G^{(1)}_{\omega_n,\mathbf{k}} \tag{5.33a}$$

$$G^{(0)}_{\omega_n,\mathbf{k}} = T_{\mathbf{k}} B^{-1}_{\omega_n,\mathbf{k}} T^\dagger_{\mathbf{k}} \tag{5.33b}$$

$$G^{(1)}_{\omega_n,\mathbf{k}} = T_{\mathbf{k}}\delta_{\mathbf{k}} B^{-1}_{\omega_n,\mathbf{k}} T^\dagger_{\mathbf{k}} - T_{\mathbf{k}} B^{-1}_{\omega_n,\mathbf{k}}\delta_{\mathbf{k}} T^\dagger_{\mathbf{k}} \tag{5.33c}$$

5.4 Mean field equations

Use the same techniques for derivatives as Eq. (4.12), we derive two saddle point equations for Δ_1 and Δ_2 from Eq. (5.20),

$$\frac{\delta}{\delta\Delta_1}: \qquad (\tilde{U}^{-1})_{11}\bar{\Delta}_1 + (\tilde{U}^{-1})_{21}\bar{\Delta}_2 - \mathrm{tr}\left[G_0 \cdot \begin{pmatrix} 0&1&0\\0&0&0\\0&0&0\end{pmatrix}\right] = 0 \tag{5.34}$$

$$\frac{\delta}{\delta\Delta_2}: \qquad (\tilde{U}^{-1})_{12}\bar{\Delta}_1 + (\tilde{U}^{-1})_{22}\bar{\Delta}_2 - \mathrm{tr}\left[G_0 \cdot \begin{pmatrix} 0&0&1\\0&0&0\\0&0&0\end{pmatrix}\right] = 0 \tag{5.35}$$

Taking Δ as real and constant,[5] we can find the mean field result. Eq. (5.19) can be inverted to get G. The inversion is quite tedious, but fortunately, we only need two elements of the G matrix ($G_{0\,(21)}$ and $G_{0\,(31)}$). The final mean-field equations are (For simplicity, both Δ_i's are taken as real. Please see Appendix B.2 for detail)

$$\begin{pmatrix}\Delta_1\\ \Delta_2\end{pmatrix} = \begin{pmatrix} U & Y \\ Y^* & V\end{pmatrix} \sum_{\mathbf{k}} \begin{pmatrix} h_{1\mathbf{k}} \\ h_{2\mathbf{k}}\end{pmatrix} \tag{5.36}$$

where

$$h_{1\mathbf{k}} = \left\langle \psi_{a,-\mathbf{k}}\psi_{b,+\mathbf{k}}\right\rangle = \Delta_1 \frac{E_{1\,\mathbf{k}} + \xi_{\mathbf{k}} + \eta}{(E_{1\,\mathbf{k}} + E_{2\,\mathbf{k}})(E_{1\,\mathbf{k}} + E_{3\,\mathbf{k}})} \tag{5.37}$$

$$h_{2\mathbf{k}} = \left\langle \psi_{a,-\mathbf{k}}\psi_{c,+\mathbf{k}}\right\rangle = \Delta_2 \frac{E_{1\,\mathbf{k}} + \xi_{\mathbf{k}}}{(E_{1\,\mathbf{k}} + E_{2\,\mathbf{k}})(E_{1\,\mathbf{k}} + E_{3\,\mathbf{k}})} \tag{5.38}$$

[5] When Y is not real, Δ_1 and Δ_2 cannot be both real even at the mean field level. Nevertheless, we can require one real, then the other will have a phase just to compensate the phase in Y. The final conclusion can be verified still valid.

Comparing Eq. 5.36 with the gap equation for the single-channel crossover, we see that $\Delta_{1,2}$ are direct counterpart of the order parameter Δ in the single-channel problem. $h_{1\mathbf{k}}$ and $h_{2\mathbf{k}}$ are the equal-time expectation of the anomalous Green's function for the open- and closed-channel. On the other hand, they correspond the macroscopic eigen-function of the two-body density matrix as described by Zhang and Leggett [Zhang, 2009, Zhang and Leggett, 2009] (see Sec. 2.3). For the purpose of many calculations, they are just like the two-body wave function. And indeed, they coincide with the two-body wave function at high momentum. We will reference them often as the "two-body correlation" in the following. If we simply take E_i to the lowest order of ζ, and ignore the closed-channel, it is easy to identify $h_{1\mathbf{k}} \approx \Delta_1/(2E_{\mathbf{k}})$ as the many-body wave function $F_{\mathbf{k}}$ in the single channel BEC-BCS crossover problem.

At high-momentum, both $h_{1\mathbf{k}}$ and $h_{2\mathbf{k}}$ behave as $1/\epsilon_{\mathbf{k}}$ which makes the summation (or the converted integral) diverges in 3D. This divergence can be mitigated by setting a high-momentum cutoff in integral or recognizing the decay of interaction in high momentum. It is important to recognize that this divergence is not unique in many-body and exists in the two-body physics, where high-momentum component of wave function is $1/\epsilon_{\mathbf{k}}$ asymptotically as well. In the next section, we proceed to remove divergence of summation in $h_{1\mathbf{k}}$ and $h_{2\mathbf{k}}$ by noting the same divergence in the two-body wave function and manipulating accordingly.

5.4.1 Renormalization of the mean field equations

The mean-field equations (Eq. 5.36) can be rewritten as

$$\Delta_{1\mathbf{p}} = \sum_{\mathbf{k}} U_{\mathbf{pk}} h_{1\mathbf{k}} + \sum_{\mathbf{k}} Y_{\mathbf{pk}} h_{2\mathbf{k}} \tag{5.39}$$

$$\Delta_{2\mathbf{p}} = \sum_{\mathbf{k}} Y_{\mathbf{pk}} h_{1\mathbf{k}} + \sum_{\mathbf{k}} V_{\mathbf{pk}} h_{2\mathbf{k}} \tag{5.40}$$

The first thing to notice is that we restore the momentum dependence of the interaction as well as of $\Delta_{1\mathbf{p}}$ and $\Delta_{2\mathbf{p}}$. Here $\Delta_{1\mathbf{p}}$ and $\Delta_{2\mathbf{p}}$ vary slowly in low momentum and it is a good approximation to take them as constant if we only study the low momentum properties. We introduce the momentum-dependence in order to gain proper convergence in summation in high momentum. As pointed out previously, both $h_{1\mathbf{k}}$ and $h_{2\mathbf{k}}$ approach $1/\epsilon_{\mathbf{k}}$ in high momentum asymptotically. This makes all summations diverge at high momentum when they are converted to integral in 3D if we take the interaction as contact and pull them out of the summation. However, we note that the real potential is not the contact-type and decays in high momentum. One way to remove the divergence is to introduce a cutoff at high-momentum while keeping the interaction coefficient constant. However, an arbitrary cutoff is undesirable for a theory. Alternatively, we can remove the divergence by restoring the momentum dependence in the interaction and recognizing

its decay at high-momentum. The problem here is that those microscopic bare interactions are hard to pin down. More readily available and observable is the two-body low-energy effective scattering matrix, T, which effectively integrates out the high-momentum component of the bare interaction. In the single channel problem, (Sec. 4.1), we introduce a relation involving the two-body s-wave scattering length a_s, (or T_0), Eq. (4.17), which has the similar divergence in high momentum. We subtract it from the summation and the remaining difference does not diverge in high momentum. A cutoff or bare momentum-dependent interaction is then no longer necessary. In principle, we can do the same in two channels and introduce the two-channel equivalent of the s-wave scattering length, a 2×2 scattering amplitude matrix. However, this 2×2 matrix is awkward in definition and not clear for the physical meaning. Therefore, we adopt a two-step process with better physical intuition behind it.

Besides the assumption of short-range potentials, we make another assumption: the two-body closed-channel bound-state at resonance, ϕ_0, is much smaller in size (a_c) than the interparticle distance (a_0), although it is larger than the potential range (r_c), $r_c \ll a_c \ll a_0$. The problem would be a genuine 3-species problem and requires other techniques if the closed-channel bound-state is about the size or even larger than the interparticle distance. As discussed at the beginning of this chapter, this assumption guarantees that the closed-channel two-body correlation $h_{2\mathbf{k}}$ follows its two-body bound-state wave function in high momentum, and we can write it as

$$h_{\mathbf{k}} \sim \phi_{0\mathbf{k}} f(\mathbf{k}) \tag{5.1}$$

with the factor $f(\mathbf{k})$ encapsulating all the many-body effects. This replacement also helps to cure the divergence involving $h_{2\mathbf{k}}$ because $\phi_{0\mathbf{k}}$ decays fast enough in high momentum and gives no singularity when integrated with the momentum-dependent interaction. After $h_{2\mathbf{k}}$ is taken care of, we proceed to remove the singularity of integral involving the open-channel two-body correlation $h_{1\mathbf{k}}$ using the regular method by subtracting the open-channel low-energy two-body interacting kernel, or the open-channel s-wave scattering length, $a_s^{(o)}$, which involves the same high-momentum divergence as $h_{1\mathbf{k}}$.

Let us put the above qualitative statement into concrete mathematical formulas. As discussed before, we start with the closed-channel correlation $h_{2\mathbf{k}}$ (Eq. 5.38). In the lowest order of ζ, we have $\frac{E_{1\,\mathbf{k}}+\xi_{\mathbf{k}}}{E_{1\,\mathbf{k}}+E_{2\,\mathbf{k}}} \approx u_{\mathbf{k}}^2$, $h_{2\mathbf{k}}$ can be rewritten into such form

$$h_{2\mathbf{k}} \approx \frac{\Delta_{2\mathbf{k}}}{(E_{1\,\mathbf{k}} + E_{3\,\mathbf{k}})} u_{\mathbf{k}}^2 \tag{5.41}$$

Here $\frac{1}{(E_{1\,\mathbf{k}}+E_{3\,\mathbf{k}})} \approx \frac{1}{2\xi_{\mathbf{k}}+\eta}$ is just the same as two-body wave function ϕ_0 besides normalization (when $k \ll \kappa$); while the extra factor $u_{\mathbf{k}}^2$ is the many-body factor $f(\mathbf{k})$ in Eq. 5.1 which describes the Pauli exclusion between two channels. At the low-momentum, the open-channel weight is large, the phase space left for

the closed-channel is limited, which is shown mathematically as a small $u_{\mathbf{k}}^2$ factor. At higher momentum ($k_F \ll k \ll 1/r_c$), there is almost nothing in the open-channel, indicated by $u_{\mathbf{k}}^2 \approx 1$ and thus the closed-channel wave-function just follows its two-body counterpart with a different normalization factor. It is not hard to see that Δ_2 is closely related to the "*integrated contact intensity*", C, in Tan's work about universality ([Tan, 2008a, Tan, 2008b]). In his work, Tan concluded that the high-end of the relative-momentum distribution asymptotically approaches C/k^4. Note that the high-end in his paper means momentum lower than $1/r_c$, but higher than any other scales ($1/a_s$, $1/a_0$). In such scale, $u_k^2 \approx 1$, $C = \frac{\Delta_2^2}{4m^2}$ for the closed-channel. At even higher momentum ($> 1/r_c$), the mean-field / saddle-point solution no longer applies. And the two-body correlation, $h_{2\mathbf{k}}$, should just follow two-body wave function (See Sec. 2.3). By all the above arguments, we replace $\frac{\Delta_2}{(E_{1\,\mathbf{k}}+E_{3\,\mathbf{k}})}$ with a normalization factor, α, and the two-body wave function $\phi_{0\mathbf{k}}$ in Eq. 5.41,

$$h_{2\mathbf{k}} = \alpha\phi_{0\mathbf{k}}u_{\mathbf{k}}^2 \tag{5.42}$$

where ϕ_0 is the normalized solution of two-body Schrödinger equation, $\sum_{\mathbf{k}} |\phi_{0\mathbf{k}}|^2 = 1$.

$$-E_b^{(0)}\phi_{0\,\mathbf{p}} = 2\epsilon_{\mathbf{p}}\phi_{0\,\mathbf{p}} - \sum_{\mathbf{k}} V_{\mathbf{pk}}\phi_{0\,\mathbf{k}} \tag{5.43}$$

By replacing $h_{2\mathbf{k}}$ with the two-body wave function at high momentum, we ignore the Pauli exclusion between different closed-channel bound-states, ϕ_0, while keeping Pauli exclusion between channels through the factor u_k^2. The higher order correction in this replacement is probably comes in as nonliner relationship between $h_{2\mathbf{k}}$ and $\phi_{0\mathbf{k}}$ or extra terms ϕ_i in expansion of $h_{2\mathbf{k}}$. However, as we will show, $h_{2\mathbf{k}}$ is always much smaller than 1. These higher order correction is relatively minor and only modifies the conclusion quantitatively without affecting the result qualitatively. Furthermore, this replacement also solves the renormalization problem automatically because the two-body wave function decays fast enough at high momentum combined with the momentum-dependent interactions and therefore we have no more divergence in integration.

Eq. 5.42 can also be understood in terms of BCS-type anstaz $\prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}}a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + w_{\mathbf{k}}a_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger\right)|0\rangle$ (Eq. 5.2) which connects to coherent states of the two-body wave function (Eq. 5.3), $\phi^{(ab)} + \phi^{(ac)}$. It is not hard to show $h_{2\mathbf{k}} = \langle a_{\mathbf{k}}c_{-\mathbf{k}}\rangle = u_{\mathbf{k}}w_{\mathbf{k}}$ for this ansatz. Using the relation $\phi_{\mathbf{k}}^{(ac)} = w_{\mathbf{k}}/u_{\mathbf{k}}$(Eq. 5.5), we have

$$h_{2\mathbf{k}} = u_{\mathbf{k}}w_{\mathbf{k}} = u_{\mathbf{k}}^2(\frac{w_{\mathbf{k}}}{u_{\mathbf{k}}}) \propto u_{\mathbf{k}}^2\phi_{\mathbf{k}}^{(ac)} \tag{5.44}$$

In a two-body problem of the Feshbach resonance, we expect $\phi^{(ac)} \propto \phi_0$ (see Chapter 3). And we have

$$h_{2\mathbf{k}} \propto \phi_{0\mathbf{k}} u_{\mathbf{k}}^2 \tag{5.45}$$

just like Eq. 5.42.

To the first order of ζ, $\phi_{0\mathbf{k}} \sim \frac{1}{\kappa^2+k^2}$, where κ is the momentum scale related to the binding energy or the tuning, $\kappa^2/2m = E_b \approx \eta$. In the many-body relevant region where momentum is not significantly larger than the Fermi momentum, this quantity is actually very small and approximately a constant, $\frac{1}{\kappa^2}$, because $\kappa \gg k_F$. The part where the many-body factor $u_{\mathbf{k}}^2$ significantly alters the wave function is actually rather small comparing to the whole spread of the wave function over the momentum space, in the order of κ ($E_b = \hbar^2\kappa^2/2m$). Within the range where $u_{\mathbf{k}}^2$ differs from 1 significantly, the wave function $\phi_{0\mathbf{k}}$ is very small. (See Appendix B.5)

$$|\phi_{0\,k=0}|^2 N \sim \left(\sqrt{\frac{\kappa}{\mathcal{V}_0}}\frac{1}{\kappa^2}\right)^2 \frac{\mathcal{V}_0}{a_0^3} = \frac{1}{(a_0\kappa)^3} \gg 1$$

This fact is valid across the full range of the crossover. At some regions of crossover, $\Delta_{2\mathbf{k}}$ (or α) may be large and the total closed-channel weight is comparable or even larger than that of the open-channel. However, for each energy level in low momentum, the factor $\phi_{0\mathbf{k}}$ is so small that the product of $h_{2\mathbf{k}}$ is still much smaller than 1. In summary, *the full closed-channel (including normalization) is always small in the low momentum region even when the total closed-channel weight is large.* This justifies our following perturbative treatment on the inter-channel Pauli exclusion between two channels.

Not far away from the resonance point, absolute detuning η is always close to binding energy $E_b^{(0)}$ of the closed-channel bound-state, ϕ_0. Using Eq. 5.41, we can write

$$\Delta_{2\mathbf{k}} = h_{2\mathbf{k}} \frac{(E_{1\mathbf{k}} + E_{3\mathbf{k}})}{u_{\mathbf{k}}^2} \approx h_{2\mathbf{k}} \frac{(E_{\mathbf{k}} + \xi_{\mathbf{k}} + \eta)}{u_{\mathbf{k}}^2}$$

Combining the above equation with Eq. 5.40, we have

$$h_{2\mathbf{k}} \frac{(E_{\mathbf{k}} + \xi_{\mathbf{k}} + \eta)}{u_{\mathbf{k}}^2} = \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'} + \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} h_{2\mathbf{k}'}$$

We replace $h_{2\mathbf{k}}$ with $\alpha u_{\mathbf{k}}^2 \phi_{\mathbf{k}}$ as in Eq. 5.42. The above equation becomes

$$\begin{aligned}
\alpha\phi_{\mathbf{k}}(E_{\mathbf{k}} + \xi_{\mathbf{k}} + \eta) &= \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'} + \alpha \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}'}^2 \phi_{\mathbf{k}'} \\
&= \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'} - \alpha \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} v_{\mathbf{k}'}^2 \phi_{\mathbf{k}'} + \alpha \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \phi_{\mathbf{k}'}
\end{aligned}$$

The last term can be rewritten as $\sum_{\mathbf{k}} V_{\mathbf{pk}}\phi_{0\,\mathbf{k}} = (2\epsilon_{\mathbf{p}} + E_b)\phi_{0\,\mathbf{p}}$ using the two-body Schrödinger equation of the isolated closed-channel Eq. 5.43. We move the last two terms from r.h.s to l.h.s, and using $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$

$$\alpha\phi_{\mathbf{k}}\left(-E_b + \eta - 2\mu + E_{\mathbf{k}} - \xi_{\mathbf{k}} + \sum_{\mathbf{k}'} V_{\mathbf{kk}'} v_{\mathbf{k}'}^2 \phi_{\mathbf{k}'}\right) = \sum_{\mathbf{k}'} Y_{\mathbf{kk}'} h_{1\mathbf{k}'}$$

Multiply both sides with $\phi_{\mathbf{k}}^*$ and integrate over the momentum,

$$\alpha\left[-E_b + \eta - 2\mu + \sum_{\mathbf{k}} \phi_{\mathbf{k}}^*(E_{\mathbf{k}} - \xi_{\mathbf{k}})\phi_{\mathbf{k}} + \sum_{\mathbf{kk}'} \phi_{\mathbf{k}}^* v_{\mathbf{k}'}^2 V_{\mathbf{kk}'}\phi_{\mathbf{k}'}\right] = \sum_{\mathbf{kk}'} \phi_{\mathbf{k}}^* Y_{\mathbf{kk}'} h_{1\mathbf{k}'} \tag{5.46}$$

We rewrite this equation in the form

$$\alpha = \frac{\sum_{\mathbf{kk}'} \phi_{\mathbf{k}}^* Y_{\mathbf{kk}'} h_{1\mathbf{k}'}}{(-E_b + \eta - 2\mu - \lambda_1)} \tag{5.47}$$

$$\lambda_1(\eta) \equiv -\sum_{\mathbf{k}} \phi_{\mathbf{k}}^*(E_{\mathbf{k}} - \xi_{\mathbf{k}})\phi_{\mathbf{k}} - \sum_{\mathbf{kk}'} \phi_{\mathbf{k}}^* v_{\mathbf{k}'}^2 V_{\mathbf{kk}'}\phi_{\mathbf{k}'} \tag{5.48}$$

Comparing this to the two-body problem Eq. 3.6, detuning is shifted by the many-body effects μ (mostly due to the Pauli exclusion within the open-channel) and λ_1 (mostly due to the Pauli exclusion between channels). λ_1 depends on detuning η (through $E_{\mathbf{k}}$, $v_{\mathbf{k}}$), but the dependence is rather weak because the integration is over mostly the short-range quantities and insensitive to the detuning. We will discuss more detail about it later in Sec 5.4.2. Using Eq. 5.47, we can express the α in $h_{2\mathbf{k}}$ (Eq. 5.42), and then plug it into Eq. 5.37

$$\Delta_{1\mathbf{p}} = \sum_{\mathbf{k}} U_{\mathbf{pk}} h_{1_{\mathbf{k}}} + \sum_{\mathbf{p}'} Y_{\mathbf{pp}'}\alpha\phi_{\mathbf{p}'} u_{\mathbf{p}'}^2 = \sum_{\mathbf{k}} U_{\mathbf{pk}} h_{1_{\mathbf{k}}} + \frac{\sum_{\mathbf{kk}'\mathbf{p}'} Y_{\mathbf{pp}'}\phi_{\mathbf{p}'}\phi_{\mathbf{k}'}^* Y_{\mathbf{kk}'} u_{\mathbf{p}'}^2 h_{1\mathbf{k}}}{(-E_b + \eta - 2\mu - \lambda_1)}$$

Comparing this with the two-body problem, we can see that the detuning part (denominator of the second term) is shifted by $2\mu + \lambda_1$ and there is an extra $u_{\mathbf{p}'}^2$ term introduced as the many-body effect. Nevertheless, none of these affect the high-momentum behavior. Therefore, the equation can be renormalized exactly as in the single-channel problem by introducing the long-wave-length s-wave scattering length a_s. We rewrite the above equation

$$\begin{aligned}\Delta_{1\mathbf{p}} = &\sum_{\mathbf{k}} \left(U_{\mathbf{pk}} + \frac{\sum_{\mathbf{k}'\mathbf{p}'} Y_{\mathbf{pp}'}\phi_{\mathbf{p}'}\phi_{\mathbf{k}'}^* Y_{\mathbf{kk}'}}{(-E_b + \eta - 2\mu - \lambda_1)}\right) h_{1\mathbf{k}} \\ &- \frac{\sum_{\mathbf{kk}'\mathbf{p}'} Y_{\mathbf{pp}'}\phi_{\mathbf{p}'}\phi_{\mathbf{k}'}^* Y_{\mathbf{kk}'} v_{\mathbf{p}'}^2 h_{1\mathbf{k}}}{(-E_b + \eta - 2\mu - \lambda_1)}\end{aligned}$$

The second term in the r.h.s. has no divergence at high momentum in 3D due to the extra $v_{p'}^2$ factor. Actually

the factor, $v_{p'}^2$, decreases quickly over a small range in the order of "gap" $\Delta_{1\mathbf{p}}$; therefore, the summation in the second term is essentially only over low-momentum, and is very small. In addition, considering the short-range nature for $Y_{\mathbf{pp'}}$, this term varies slowly over momentum, $\mathbf{p}$.

Multiply both side with $(1+TG)$, where T is the scattering matrix for the open-channel, and $G = (\omega - H_0)^{-1}$ is the Green's function for a free pair in the open-channel.[6]

$$(1+TG)\Delta_1 = -Th_1 - \lambda_2$$

$$\lambda_{2\mathbf{p}} \equiv \sum_{\tilde{\mathbf{p}}}(1+TG)_{\mathbf{p}\tilde{\mathbf{p}}}\frac{\sum_{\mathbf{kk'p'}} Y_{\tilde{\mathbf{p}}\mathbf{p'}}\phi_{\mathbf{p'}}\phi^*_{\mathbf{k'}}Y_{\mathbf{kk'}}v^2_{\mathbf{p'}}h_{1_{\mathbf{k}}}}{(-E_b+\eta-2\mu-\lambda_1)} = \alpha\sum_{\tilde{\mathbf{p}}\,\mathbf{p'}}(1+TG)_{\mathbf{p}\tilde{\mathbf{p}}}Y_{\tilde{\mathbf{p}}\mathbf{p'}}\phi_{\mathbf{p'}}v^2_{\mathbf{p'}} \tag{5.49}$$

In principle, $\lambda_{2\mathbf{p}}$ depends on momentum, however, like $\Delta_{1\mathbf{p}}$, it is approximately constant at low momentum. We are only interested in the low momentum/frequency properties as the system is cold, dilute and governed by only short-range interactions. The scattering matrix T is approximately its s-wave zero-energy value $4\pi\tilde{a}_s(\mu,\lambda_1)/m$ although $\tilde{a}_s(\mu,\lambda_1)$ is the s-wave scattering length of the shifted (by $2\mu+\lambda_1$) detuning. The s-wave scattering length, a_s, in the two-body problem without many-body shift $2\mu+\lambda_1$ is simply Eq. 3.13.

$$a_s(\delta) = a_{bg}\left(1+\frac{\mathcal{K}}{\delta}\right) \tag{3.13}$$

Here in the many-body context with the extra detuning $2\mu+\lambda_1$, $\tilde{a}_s$ is

$$\tilde{a}_s = a_{\mathrm{bg}}(1+\frac{\mathcal{K}}{\delta-2\mu-\lambda_1}) \tag{5.50}$$

where $\mathcal{K}$ is introduced in Eq. 3.12 of Chapter 3. The Green's function is simply $1/2\epsilon_{\mathbf{k}}$ at zero energy. Similarly, $\Delta_{1\mathbf{p}}$ and $\lambda_{2\mathbf{p}}$ is approximately constant at low momentum. We drop the subscript $\mathbf{p}$ of them, and pull Δ_1 out of summation.

$$\Delta_1 = -T\sum(h_1+G\Delta_1)-\lambda_2 = -\frac{4\pi\tilde{a}_s(\mu,\lambda_1)}{m}\Delta_1\sum(\frac{E_{1\,\mathbf{k}}+\xi_{\mathbf{k}}+\eta}{(E_{1\,\mathbf{k}}+E_{2\,\mathbf{k}})(E_{1\,\mathbf{k}}+E_{3\,\mathbf{k}})}-\frac{1}{2\epsilon_{\mathbf{k}}})-\lambda_2 \tag{5.51}$$

Here the last step use the zero energy value of the zero-energy free pair Green's function $G(\omega=0) = (-2\epsilon_{\mathbf{k}})^{-1}$. Dividing both sides with Δ_1, we have the renormalized equation

$$1 = -\left[\frac{4\pi\tilde{a}_s(\mu,\lambda_1)}{m}\sum(\frac{E_{1\,\mathbf{k}}+\xi_{\mathbf{k}}+\eta}{(E_{1\,\mathbf{k}}+E_{2\,\mathbf{k}})(E_{1\,\mathbf{k}}+E_{3\,\mathbf{k}})}-\frac{1}{2\epsilon_{\mathbf{k}}})\right]-\frac{\lambda_2}{\Delta_1} \tag{5.52}$$

[6]Here we use the relation of the scattering T-matrix, the free pair Green's function $G=(\omega-H_0)^{-1}$ and the bare interaction $V=-U_{\mathrm{eff}}$.

$$T = V+TGV = -(1+TG)U_{\mathrm{eff}}$$

Note that $\tilde{a}_s(\mu, \lambda_1)$ corresponds to the two-body s-wave scattering length at detuning shifted by $2\mu + \lambda_1$.

Now we can expand the first term in the parentheses to the first order of ζ, using Eq. 5.28. Keeping in mind $E_{\mathbf{k}} \ll \eta$ at low momentum where summation is about, we have[7]

$$1 = -\left[\frac{4\pi\tilde{a}_s(\mu, \lambda_1)}{m}\sum(\frac{1}{2E_{\mathbf{k}}} - \frac{1}{2\epsilon_{\mathbf{k}}} - \frac{\Delta_2^2\xi_{\mathbf{k}}}{4(\xi_{\mathbf{k}}+\eta)E_{\mathbf{k}}^3})\right] - \frac{\lambda_2}{\Delta_1} \tag{5.53}$$

The correction term (the third term in parentheses) does not have divergence in summation of high-momentum. In summary, there are several difference of gap equation here comparing to single-channel problems:

1. The shift of 2μ in detuning through $\tilde{a}_s$;
2. The extra shift of λ_1 (see Eq. 5.48) in detuning through $\tilde{a}_s$;
3. The extra term $-\frac{\lambda_2}{\Delta_1}$ in Eq. 5.53;
4. The extra term $-\frac{\Delta_2^2\xi_{\mathbf{k}}}{4(\xi_{\mathbf{k}}+\eta)(E_{\mathbf{k}})^3} \approx -\frac{\xi_{\mathbf{k}}\Delta_1}{4E_{\mathbf{k}}^3}\zeta$ in the summation of Eq. 5.53;

Item 1 corresponds to a many-body effect common to both three and four species problem. In a many-body system, most of the properties can obtained when considering what happens at the next extra particle or particle pair. In a two-body system, we can pretend that the vacuum is the initial state and the next particle pair comes in from energy zero. In a many-body system, this starting point is no longer the absolutely zero, but the chemical potential. Excitations are counted from the chemical potential, μ. The energy detuning in Feshbach resonance is no exception. In a many-body formula, the detuning is shifted by 2μ (for a pair). In the broad resonance, the Fermi energy is smaller comparing to the detuning during the relevant probing region. Consequently, this shift is negligible. In the narrow resonance, the Fermi energy, however, is substantial and a detuning of the chemical potential needs to be taken into account. At the BCS side, μ is positive and close to the Fermi energy. This shifting just confirms the fact that most interesting phenomenon in a fermion system happens around Fermi surface instead of absolute zero. With an extra positive shift μ, detuning is reduced; therefore the crossover region is actually reached earlier (i.e. by larger detuning) than in two-body cases. On the other hand, moving toward to the resonance point and BEC side, the chemical potential becomes smaller and finally flips sign to negative. Accordingly, the detuning is reduced lesser and lesser; finally it is enhanced. Interestingly, the crossing point, $\mu = 0$, is not shifted from a model with simple s-wave scattering length directly from two-body physics if only considering this shift (See Fig. 5.2). This effect is also studied extensively previously. (Sec. 6.2 of [Gurarie and Radzihovsky, 2007]).

[7]Here we used $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}$

The next three corrections are unique for three-species problem where the inter-channel Pauli exclusion cannot be neglected. Furthermore, close look into λ_1 and λ_2 (Sec. 5.4.2) reveals that they vary slowly across the full region of crossover and are functions of the density of atoms in the open-channel . They describe fundamental many-body effects, and do not have counterparts in a two-body problem. Both λ_1 (see Eq. 5.48) and λ_2 (see Eq. 5.49) involve overlap integrals between the open-channel wave function and the closed-channel wave function, (factor $v_{\mathbf{k}}^2$ or $u_{\mathbf{k}}^2$ describes mostly the open-channel wave function; while ϕ describes the closed-channel wave function). The larger the overlap of the two, the larger λ_1 and λ_2 are. This has a very intuitive interpretation: more overlap leads more severe inter-channel Pauli exclusion, which in turn leads to larger λ_1 and λ_2 that describe this effect between two channels. In our model, an open-channel wave function is spread all over the real-space, (even at BEC-side, the real bound-state is very loosely bound comparing to the closed-channel bound state), while the closed-channel wave function is very sensitive to the binding energy, $E_b(\approx \eta)$. When the closed-channel bound-state is closer to the threshold, i.e., the binding energy is smaller, the closed-channel bound-state is more spread out in real space and has larger overlap with open-channel. Consequently, λ_1 and λ_2 are larger in such cases. Nevertheless, λ_1 is much smaller than the Fermi energy E_F, or the other shift, the chemical potential, 2μ. So the shift is not very large and it is still all right to treat it as a perturbation. The correction is shifted with the change of the density. In the many-body system, no dramatic jump in physical quantities happens at resonance due to the crossover nature, and it is hard to observe this shift over the resonance position though.

5.4.2 Evaluation and estimation of λ_1 and λ_2

From the last section, we see that a lot of the inter-channel Pauli exclusion is encapsulated in two parameters λ_1 and λ_2. Therefore, it is well-worthwhile to study them in more details. λ_1 is defined as

$$\lambda_1(\eta) \equiv -\sum_{\mathbf{k}} \phi_{\mathbf{k}}^*(E_{\mathbf{k}} - \xi_{\mathbf{k}})\phi_{\mathbf{k}} - \sum_{\mathbf{k}\mathbf{k}'} \phi_{\mathbf{k}}^* v_{\mathbf{k}'}^2 V_{\mathbf{k}\mathbf{k}'}\phi_{\mathbf{k}'} \tag{5.48}$$

Use relationship $v_k^2 = \frac{E_{\mathbf{k}} - \xi_{\mathbf{k}}}{2E_{\mathbf{k}}}$, we can rewrite the above equation into

$$\lambda_1(\eta) \equiv -\sum_{\mathbf{k}} \phi_{\mathbf{k}}^* v_{\mathbf{k}}^2 (2E_k\phi_{\mathbf{k}} + \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\phi_{\mathbf{k}'}) \tag{5.54}$$

We can then replace the second term in the parentheses using the two-body Schrödinger equation of the isolated closed-channel Eq. 5.43, $\sum_{\mathbf{k}} V_{\mathbf{pk}}\phi_{\mathbf{k}} = (E_b + 2\epsilon_{\mathbf{p}})\phi_{\mathbf{p}}$.

$$\lambda_1(\eta) = -\sum_{\mathbf{k}} \phi^*_{\mathbf{k}} v^2_{\mathbf{k}} \left[2(E_k + \epsilon_k) + E_b\right] \phi_{\mathbf{k}} \approx \sum_{\mathbf{k}} \left|\phi_{\mathbf{k}}\right|^2 v^2_{\mathbf{k}} \left[2\left(E_k + \epsilon_k\right) + \eta\right]$$

In the above summation, $v^2_{\mathbf{k}}$ is only non-zero below or not much higher than the Fermi momentum. In this range, $E_{\mathbf{k}}, \epsilon_{\mathbf{k}} \ll \eta$ and we can neglect $E_{\mathbf{k}} + \epsilon_{\mathbf{k}}$ comparing to η. Furthermore, $\phi_{\mathbf{k}}$ varies slowly in this range, because the closed-channel bound state is much smaller than the interparticle distance. It is a good approximation to replace $\phi_{\mathbf{k}}$ with $\phi_{\mathbf{k}=0} \approx \frac{A}{\kappa^2}$ and to take it out of the summation. Put all these together, we can estimate λ_1

$$\lambda_1 \approx -\eta \left|\phi_{k=0}\right|^2 \sum v^2_{\mathbf{k}} = -\eta \left|\phi_{k=0}\right|^2 N_o \tag{5.55}$$

where N_o is the total number of atoms in the open-channel. It is easy to see that $|\lambda_1|$ is much smaller than η as $\left|\phi_{k=0}\right|^2 N_o \ll 1$. Furthermore, using $\phi_{k=0} \approx \sqrt{\frac{8\pi\kappa}{\mathcal{V}_0}} \frac{1}{\kappa^2}$ (Eq. B.13 of Appendix B.3), we get $\lambda_1 \sim \frac{a_c}{a_0} E_F \ll E_F$, where a_0 is the average interparticle distance and a_c is the size of the close-channel bound-state. We have showed that λ_1 is indeed a minor correction over shift μ. It is not easy to estimate λ_1 precisely from microscopic parameters above because these parameters themselves are in turn hard to estimate precisely. Nevertheless, a key observation is that λ_1 depends on the (open-channel) density ($n_0 = \mathcal{V}_0^{-1} \sum_{\mathbf{k}} v^2_{\mathbf{k}}$) linearly to the lowest order of $\frac{a_c}{a_0}$,

$$\lambda_1 \approx \lambda_1^{(0)} n_o \tag{5.56}$$

We can perform the experiments at different densities and estimate the coefficient $\lambda_1^{(0)}$.

λ_2 is defined as

$$\lambda_{2\mathbf{p}} \equiv \sum_{\tilde{\mathbf{p}}} (1 + TG)_{\mathbf{p}\tilde{\mathbf{p}}} \frac{\sum_{\mathbf{k}\mathbf{k}'\mathbf{p}'} Y_{\tilde{\mathbf{p}}\mathbf{p}'} \phi_{\mathbf{p}'} \phi^*_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} v^2_{\mathbf{p}'} h_{1_{\mathbf{k}}}}{(-E_b + \eta - 2\mu - \lambda_1)} = \alpha \sum_{\tilde{\mathbf{p}}\,\mathbf{p}'} (1 + TG)_{\mathbf{p}\tilde{\mathbf{p}}} Y_{\tilde{\mathbf{p}}\mathbf{p}'} \phi_{\mathbf{p}'} v^2_{\mathbf{p}'} \tag{5.49}$$

Here the argument goes similar as in the λ_1 case, considering the short-range nature, both $Y_{\tilde{\mathbf{p}}\mathbf{p}'}$ and $\phi_{\mathbf{p}'}$ vary slowly and can be approximated by their value at $\mathbf{p}' = 0$ for the momentum below or around the Fermi momentum. After pulling these two quantities out of the summation over $\mathbf{p}'$, we only need to sum over $v^2_{\mathbf{p}'}$, which gives a familiar factor, the (open-channel) density, n_o. In addition, $\alpha = \sqrt{n_c}$. The factor $(1 + TG)_{\mathbf{p}\tilde{\mathbf{p}}}$ integrate out the high momentum component and $\lambda_{2\mathbf{p}}$ is close to a constant at low momentum $\mathbf{p}$. We have

$$\lambda_2 \approx \lambda_2^{(0)} n_o \sqrt{n_c} \tag{5.57}$$

In experiments, λ_1 and λ_2 can be measured at different total densities. The two coefficients, $\lambda_1^{(0)}$ and $\lambda_2^{(0)}$, which do not depend on the density, can then be estimated according to Eqs. 5.56 and 5.57.

5.4.3 Number equations

There is one number equation for each channel,

$$\sum_{\omega_n,\mathbf{k}} G_{22} e^{(-i\omega_n \delta_-)} = N_{open}$$
$$\sum_{\omega_n,\mathbf{k}} G_{33} e^{(-i\omega_n \delta_-)} = N_{close}$$

Note that the Matsubara summation formally diverges and we need to put in a small negative part into the summation in order to prevent the divergence. Here we put in a small negative part instead of a positive part because Ψ_2 and Ψ_3 are conjugate of real particles, $\Psi_2 = \bar{\psi}_b$, $\Psi_3 = \bar{\psi}_c$. The Matsubara summation can be performed with the normal trick of multiplying a Fermi function to summand and deform the contour (see Appendix B.2 for more details). For the summation at zero temperature, we just need to consider the positive roots, $E_{1\,\mathbf{k}}$. It is straightforward to find

$$N_{\text{open}} = \sum_{\mathbf{k}} \frac{(E_{1\,\mathbf{k}} - \xi_{\mathbf{k}})(E_{1\,\mathbf{k}} + \xi_{\mathbf{k}} + \eta) - \Delta_2^2}{(E_{1\,\mathbf{k}} + E_{2\,\mathbf{k}})(E_{1\,\mathbf{k}} + E_{3\,\mathbf{k}})} \tag{5.58}$$

$$N_{\text{closed}} = \sum_{\mathbf{k}} \frac{(E_{1\,\mathbf{k}} - \xi_{\mathbf{k}})(E_{1\,\mathbf{k}} + \xi_{\mathbf{k}}) - \Delta_1^2}{(E_{1\,\mathbf{k}} + E_{2\,\mathbf{k}})(E_{1\,\mathbf{k}} + E_{3\,\mathbf{k}})} = \sum_{\mathbf{k}} \frac{E_{1\,\mathbf{k}}^2 - E_{\mathbf{k}}^2}{(E_{1\,\mathbf{k}} + E_{2\,\mathbf{k}})(E_{1\,\mathbf{k}} + E_{3\,\mathbf{k}})} \tag{5.59}$$

Let us look at the equation of the closed-channel first, if we expand $E_{i\,\mathbf{k}}$ using Eqs. 5.28-5.30, the lowest order is

$$N_{\text{closed}} \approx \sum_{\mathbf{k}} \frac{\gamma_{1\,\mathbf{k}}}{(E_{\mathbf{k}} + \xi_{\mathbf{k}} + \eta)} = \sum_{\mathbf{k}} \frac{\Delta_2^2 u_{\mathbf{k}}^2}{(\xi_{\mathbf{k}} + \eta)(E_{\mathbf{k}} + \xi_{\mathbf{k}} + \eta)} \tag{5.60}$$

Here γ_1 is the correction for the fermionic correlation spectrum due to the inte-channel Pauli exclusion (Eq. 5.28). We take the full value $\frac{\Delta_2^2 u_{\mathbf{k}}^2}{(\xi_{\mathbf{k}}+\eta)}$, instead of the low-momentum value because the summation has substantial contribution from high momentum. This is consistent with Eq. 5.38 and 5.41 if we assume[8] $N_{\text{closed}} \approx \sum h_2^2$. From appendix B.5, we know that the summand is much smaller than 1 in all regions. Particular, in the low momentum ($\lesssim k_F$), the summand is $\zeta \frac{\Delta_1}{\eta} u_{\mathbf{k}}^2 \ll 1$. Nevertheless, the weight spread in a very large range of momentum ($\sim \eta$), so the resulting sum can be still in the order of total number N at certain detuning.

[8] As discussed before, in the closed-channel $h_{2\mathbf{k}} \ll 1$ over all momentum. Furthermore, the summation goes over very large momentum range, the difference between $h_{2\mathbf{k}}$ and the closed-channel particle number is only large below or around Fermi energy, but the total weight of the closed-channel atoms in such a region is very small.

Note that the connection between Δ_2 and the "Contact" in the theory of universality ([Tan, 2008a, Tan, 2008b]). The summand as density of momentum is valid at momentum up to the scale $1/a_c$, and is mostly determined by two-body physics except an overall factor at "high momentum" ($k_F \ll k \ll 1/r_c$). Furthermore, the contribution from the very high momentum ($k \gg 1/r_c$) to integral is small. All the deviation there can be absorbed as a small correction in Δ_2. To zeroth order of ζ, $E_{i\mathbf{k}} \approx \xi_{\mathbf{k}}$ and $u_{\mathbf{k}}^2 \approx 1$ for the most of the integral domain. This summation can be written as

$$N_{\text{closed}} \approx \sum_{\mathbf{k}} \frac{\Delta_2^2}{(\xi_{\mathbf{k}}+\eta)(2\xi_{\mathbf{k}}+\eta)} \tag{5.61}$$

This equation has only one unknown parameter Δ_2. Therefore, this equation can be used to estimate Δ_2 from experiments. The estimation of Δ_2 from such procedure automatically includes the correction from high momentum.

The open-channel number equation can be expanded perturbatively as well,

$$\begin{aligned} N_{\text{open}} &\approx \sum_{\mathbf{k}} \left[\frac{E_{\mathbf{k}}-\xi_{\mathbf{k}}}{2E_{\mathbf{k}}} + \frac{\gamma_{1\mathbf{k}}}{2E_{\mathbf{k}}} - \frac{(E_{\mathbf{k}}-\xi_{\mathbf{k}})(\gamma_{1\mathbf{k}}+\gamma_{2\mathbf{k}})}{4E_{\mathbf{k}}^2} - \frac{(E_{\mathbf{k}}-\xi_{\mathbf{k}})\gamma_{3\mathbf{k}}}{2E_{\mathbf{k}}(\xi_{\mathbf{k}}+E_{\mathbf{k}}+\eta)} - \frac{\Delta_2^2}{2E_{\mathbf{k}}(\xi_{\mathbf{k}}+E_{\mathbf{k}}+\eta)} \right] \\ &\approx \sum_{\mathbf{k}} \left[\frac{E_{\mathbf{k}}-\xi_{\mathbf{k}}}{2E_{\mathbf{k}}} + \frac{E_{\mathbf{k}}-\xi_{\mathbf{k}}}{2E_{\mathbf{k}}} \frac{\Delta_1}{2(E_{\mathbf{k}}+\xi_{\mathbf{k}}+\eta)} \zeta - \frac{\Delta_1^3}{4E_{\mathbf{k}}^3}\zeta \right] \end{aligned} \tag{5.62}$$

All terms behave well in 3D and do not need any renormalization. It is like the number equation in the single channel with a few correction in the order of $\zeta = \Delta_2^2/\eta\Delta_1$. The second term, except the factor $\frac{E_{\mathbf{k}}-\xi_{\mathbf{k}}}{2E_{\mathbf{k}}} = v_{\mathbf{k}}^2$, looks like the summand in the closed-channel number equation, Eq. 5.60, which can sum up in the order of N. Nevertheless, the $v_{\mathbf{k}}^2$ factor, decreases quickly in high momentum, becomes close to zero for $k \gg k_F$, and limits the summation to only low momentum. This makes the sum a small correction as we discussed before. Similarly, $\frac{\Delta_1^2}{E_{\mathbf{k}}^2}$ in the third term also limits the summation to low momentum and ensures that the sum is a small correction. At low momentum, this term is actually more important than the second term.

5.5 Discussion of the mean-field solution

As discussed before, the correction of the narrow Feshbach resonance can be taken into account in two steps. First, omitting the inter-channel Pauli exclusion, we only consider the chemical potential μ in the shift and the extra counting of the closed-channel. Then in the second step, we can correct the previous result with quantities originated from the inter-channel Pauli-exclusion unique in the three-species problem.

In the first step, the gap equation and the (open-channel) number equation are simplified to

$$1 = -\left[\frac{4\pi\tilde{a}_s(\mu)}{m}\sum(\frac{1}{2E_{\mathbf{k}}} - \frac{1}{2\epsilon_{\mathbf{k}}})\right] \tag{5.63}$$

$$N_{\text{open}} = \sum_{\mathbf{k}} \frac{E_{\mathbf{k}} - \xi_{\mathbf{k}}}{2E_{\mathbf{k}}} \tag{5.64}$$

Here we only consider the shift of the chemical potential 2μ in $\tilde{a}_s$ (Eq. 5.50),

$$\tilde{a}_s = a_{\text{bg}}(1 + \frac{\mathcal{K}}{\delta - 2\mu}) \approx \frac{a_{\text{bg}}\mathcal{K}}{\delta - 2\mu} \tag{5.65}$$

In the second equation, we assume $a_{\text{bg}} \ll a_0$ (a_0 is the average interparticle distance) and we only study situations close to resonance, where $\mathcal{K} \gg \delta \,\text{or}\, \mu$ (δ is the detuning from the resonant point in two-body physics). From the two-body analysis of the Feshbach resonance, we know the numerator in the Eq. 5.65 is closely related to the characteristic scale δ_c defined in Eq. 3.19

$$\delta_c \equiv \frac{\mathcal{K}^2}{\hbar^2/m_r a_{bg}^2} = \frac{(\mathcal{K}a_{\text{bg}})^2}{\hbar^2/m_r} \tag{3.19}$$

We can rewrite the $\tilde{a}_s$ with respect to δ_c

$$\tilde{a}_s = \frac{\sqrt{2\delta_c\hbar^2/m}}{\delta - 2\mu} \tag{5.66}$$

In the narrow resonance, the weight of the closed-channel becomes substantial quickly. We can calculate the amplitude of the closed-channel according to Eq. 5.47

$$\alpha = \frac{\sum_{\mathbf{k}\mathbf{k}'} \phi_{\mathbf{k}}^* Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'}}{(-E_b + \eta - 2\mu - \lambda_1)} \tag{5.47}$$

Y, as a short-range interaction, only picks up the short-range part of $h_1(r)$ and $\phi(r)$ in the above integral. The short-range part of h_1 is assumed to be proportional to the short-range part of the two-body wave function. Its normalization, however, comes from many-body physics. If we assume the zeroth order form, $h_1 = \Delta_1/2E_{\mathbf{k}}$, Zhang has derived the form of $h_1(\mathbf{r})$ in the real space, (Eq. (25) in [Zhang and Leggett, 2008])

$$h_1(r) = \frac{m\Delta_1}{4\pi\hbar^2}\frac{1 - r/a_s}{r} \tag{5.67}$$

Comparing this one with the Bethe-Peierls boundary condition Eq. 2.4, we find that $\frac{m\Delta_1}{4\pi\hbar^2}$ is the normalization factor. And Δ_1 is determined by the number equation for open-channel density n_0. Similar as the two-body

case (Eq. 3.21), we can write

$$\alpha^2 = \frac{\left|\sum_{\mathbf{k}\mathbf{k}'} \phi^*_{\mathbf{k}} Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'}\right|^2}{\left(-E_b + \eta - 2\mu - \lambda_1\right)^2} \tag{5.68}$$

Extracting the normalization factor of h_1, the integral in the numerator then is just the same as that in the two-body physics and can be rewritten using the expression of $\mathcal{K}$ according to Eq. 3.12.

$$\left|\sum_{\mathbf{k}\mathbf{k}'} \phi^*_{\mathbf{k}} Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'}\right|^2 = \left(\frac{m\Delta_1}{4\pi\hbar^2}\right)^2 \frac{\hbar^2\mathcal{K}}{m a_{bg}} \tag{5.69}$$

Here we use $m_r = \frac{1}{2}m$. We further assume that the energy difference between the resonant point ($a_s \to \pm\infty$) and the level crossing point, where the uncoupled closed-channel bound state level is at the threshold of the open-channel, $\mathcal{K}$, is in fact much larger than μ or δ_c, i.e. $|-E_b + \eta| \gg 2\mu, \lambda_1$. So we have $|-E_b + \eta - 2\mu - \lambda_1| \approx \mathcal{K}$ (note that here η is equivalent to $\tilde{\delta}$ in the two-body Eq. 3.23). We can then write

$$n_c \approx \frac{m\Delta_1^2}{32\pi^2\hbar^2} \frac{1}{\mathcal{K} a_{bg}} \tag{5.70}$$

From Eq. 3.19 above, we can replace $\mathcal{K}a_{bg}$ with $\sqrt{2\delta_c\hbar^2/m}$ using Eq. 3.19. After dividing both sides with the total density $n_{tot} = \left(\frac{mE_F^{(tot)}}{\hbar^2}\right)^{3/2} \frac{\sqrt{2}}{3\pi^2}$, we find the weight for the closed-channel

$$\beta_c = \frac{n_c}{n_{tota}} \approx \frac{3\sqrt{2}}{128} \frac{\Delta_1^2}{\sqrt{{E_F^{(tot)}}^3 \delta_c}} \tag{5.71}$$

β_c is proportional to Δ_1^2. This form is consistent with the formula obtained by Zhang previously [Zhang and Leggett, 2009]. In Fig. 5.2, we plot the open-channel weight

$$\beta_o = 1 - \beta_c \tag{5.72}$$

We can see an example of the narrow resonance ($\delta_c = 0.001E_F^{(tot)}$) in the Fig. 5.2. We rescale the detuning with E_0 [9]

$$E_0 = \sqrt{2\delta_c\hbar^2/m} \cdot k_F = 2\sqrt{\delta_c E_F} \tag{5.73}$$

Δ_1 saturates at about $0.8E_F$. At the BCS limit, $n_o \approx n_{tot}$, $\beta_0 \approx 1$. Δ_1 is exponentially small, there is only very small amount of atoms in the closed-channel. Moving toward the resonance and then the BEC side, Δ_1 increases and the closed-channel density increases as well. At the universality point of the two-body

[9] We choose this scale in order to make sure that $\tilde{a}_s k_F$ would match $a_s k_F$ in the single channel discussion in Chapter 4 if there was no -2μ shift as in Eq. 5.65 in order to comparing with the single channel case as in Fig. 4.1. When $\delta/E_0 = 1$, $-\tilde{a}_s k_F = 1$ if there was no extra -2μ shift.

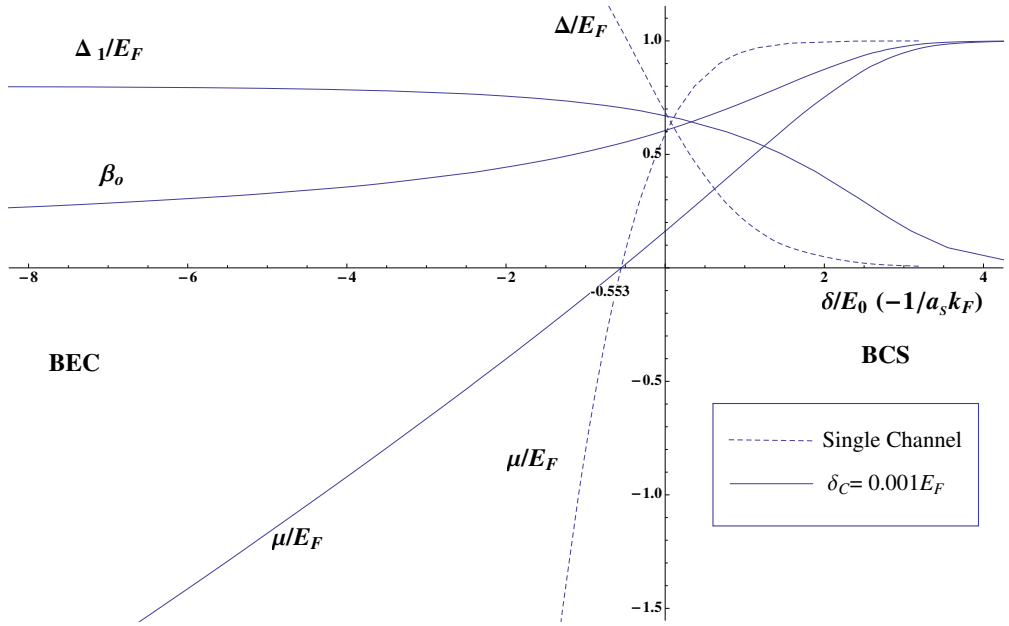


Figure 5.2: The narrow Feshbach resonance w/o the inter-channel Pauli exclusion vs. the single-channel model

We plot the chemical potential μ, the open-channel gap Δ_1 and the open-channel relative weight β_o for the narrow resonance; and chemical potential and the gap for the single-channel model. The gap in the open-channel Δ_1 and the chemical potential μ are rescaled with the the Fermi energy of the total density, $E_F^{(tot)}$. The x-axis is the detuning δ rescaled with E_0 (see Eq. 5.73) for the narrow resonance; while it is $-1/a_s k_F$ for the single-channel curves. We have taken $\delta_c = 0.001 E_F^{(tot)}$ for the narrow resonance figure. We used the detuning from the resonant point for the x-axis in the narrow resonance instead of $-1/a_s k_F$ in the single-channel because the additional shift, 2μ, considering in Eq. 5.65. Consequently, the chemical potential lines in both cases cross the x-axis at the same point where $\mu = 0$.

physics, Δ_1 is in the order of the Fermi energy, and β_o is already substantially smaller than 1 if the resonance is narrow. Because the maximum of the n_c is the total density n_{tot}, we can see that Δ_1 saturates. The narrower the resonance, the sooner it saturates.

We can understand the saturation of Δ_1 from another respect. Let us look at the open-channel gap equation Eq. 5.39

$$\Delta_{1\mathbf{p}} = \sum_{\mathbf{k}} U_{\mathbf{pk}} h_{1\mathbf{k}} + \sum_{\mathbf{k}} Y_{\mathbf{pk}} h_{2\mathbf{k}} \tag{5.39}$$

Not far away from the resonance, the second term dominates the first term. And considering Eq. 5.42, $h_{2\mathbf{k}} = \alpha\phi_{0\mathbf{k}} u_{\mathbf{k}}^2$, it is not hard to see that the closed-channel normalization factor α is proportional to Δ_1. Moving toward the BEC end from the BCS end, the closed-channel density increases as Δ_1 increases and eventually dominates the open-channel density. In fact, when the closed-channel dominates, $\alpha \approx \sqrt{N}$; consequently Δ_1 saturates and is directly proportional to the square root of the total density.

$$\Delta_1 \approx \sqrt{N} \sum_{\mathbf{k}} Y_{\mathbf{p}=0,\,\mathbf{k}} \phi_{0\mathbf{k}} u_{\mathbf{k}}^2 \approx \sqrt{n_{\mathrm{tot}}} \Delta_{1,\mathrm{sat}}^{(0)} \tag{5.74}$$

Here the coefficient $\Delta_{1,\mathrm{sat}}^{(0)}$ is common for one specific Feshbach resonance. It is possible to observe this saturation experimentally by measuring the fermionic excitation spectrum.

We have the zeroth order result, $\mu^{(0)}$, $\Delta_1^{(0)}$ from the previous step. Now we can write down mean-field equations including the inter-channel Pauli exclusion effects, expand them and look for the first order corrections, $\mu^{(1)}$ and $\Delta_1^{(1)}$. Δ_2 is a first order quantity by itself, and is related to the closed-channel density by Eq. 5.60. Therefore, we do not need to include Δ_2 when looking for the first order corrections.

We start from the open-channel gap equation (Eq. 5.53) and number equation (Eq. 5.62)

$$\frac{m}{4\pi\tilde{a}_s(\mu,\lambda_1)} = -\sum\left(\frac{1}{2E_{\mathbf{k}}} - \frac{1}{2\epsilon_{\mathbf{k}}}\right) + \sum \frac{\Delta_2^2 \xi_{\mathbf{k}}}{4(\xi_{\mathbf{k}}+\eta)E_{\mathbf{k}}^3} - \frac{m}{4\pi\tilde{a}_s(\mu,\lambda_1)}\left(\frac{\lambda_2}{\Delta_1}\right) \tag{5.75}$$

$$N_{\mathrm{open}} \approx \sum\left(\frac{1}{2} - \frac{\xi_{\mathbf{k}}}{2E_{\mathbf{k}}}\right) + \sum \frac{E_{\mathbf{k}} - \xi_{\mathbf{k}}}{2E_{\mathbf{k}}} \frac{\Delta_1}{2(E_{\mathbf{k}}+\xi_{\mathbf{k}}+\eta)}\zeta - \sum \frac{\Delta_1^3}{4E_{\mathbf{k}}^3}\zeta \tag{5.76}$$

We have rearranged these two equations to better compare them with the gap equation and the number equation used in the previous step, Eqs. 5.63 and 5.64. The main structure of the equations are the similar. In the gap equation (Eq. 5.53), the second and the third term in the r.h.s are due to the inter-channel Pauli exclusion. In addition, $\tilde{a}_s$ in the l.h.s. also has a small correction due to the shift λ_1(Eq. 5.66 and Eq. 5.50).

$$\frac{1}{\tilde{a}_s^{(0)}(\mu^{(0)})} - \frac{1}{\tilde{a}_s(\mu,\lambda_1)} = \frac{1}{\sqrt{2\delta_c\hbar^2/m}}\lambda_1 \tag{5.77}$$

We can expand the $1/(2E_{\mathbf{k}})$ with $\mu \to \mu^{(0)} + \mu^{(1)}$ and $\Delta_1 \to \Delta_1^{(0)} + \Delta_1^{(1)}$, where the zeroth order terms $\mu^{(0)}$ and $\Delta_1^{(0)}$ satisfy gap equation in the previous step, Eq. 5.63. We then get the equation for $\mu^{(1)}$ and $\Delta_1^{(1)}$.

$$\frac{m}{4\pi}\frac{\lambda_1}{\sqrt{2\delta_c\hbar^2/m}} = -\frac{1}{2}\sum\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}^3}\mu^{(1)} + \frac{1}{2}\sum\frac{\Delta_1^{(0)}}{E_{\mathbf{k}}^3}\Delta_1^{(1)} + \sum\frac{\Delta_2^2\xi_{\mathbf{k}}}{4(\xi_{\mathbf{k}}+\eta)E_{\mathbf{k}}^3} - \frac{m}{4\pi\tilde{a}_s^{(0)}(\mu,\lambda_1)}(\frac{\lambda_2}{\Delta_1}) \tag{5.78}$$

$$\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu^{(0)} \tag{5.79}$$

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_1^{(0)2}} \tag{5.80}$$

Similarly, we can expand the $\xi_{\mathbf{k}}/(2E_{\mathbf{k}})$ in the number equation with $\mu \to \mu^{(0)} + \mu^{(1)}$ and $\Delta_1 \to \Delta_1^{(0)} + \Delta_1^{(1)}$, where the zeroth order terms $\mu^{(0)}$ and $\Delta_1^{(0)}$ satisfy number equation in the previous step, Eq. 5.64. We then find the other equation for $\mu^{(1)}$ and $\Delta_1^{(1)}$.

$$0 = -\frac{1}{2}\sum\frac{\Delta_1^{(0)2}}{E_{\mathbf{k}}^3}\mu_1^{(1)} - \frac{1}{2}\sum\frac{\xi_{\mathbf{k}}\Delta_1^{(0)}}{E_{\mathbf{k}}^3}\Delta_1^{(1)} + \sum\frac{E_{\mathbf{k}}-\xi_{\mathbf{k}}}{2E_{\mathbf{k}}}\frac{\Delta_1^{(0)}}{2(E_{\mathbf{k}}+\xi_{\mathbf{k}}+\eta)}\zeta - \sum\frac{\Delta_1^{(0)3}}{4E_{\mathbf{k}}^3}\zeta \tag{5.81}$$

Please refer to Eqs. 5.48 and 5.49 as well as Sec. 5.4.2 for λ_1 and λ_2. These two quantities describe the overlapping between two channels, i.e. the inter-channel Pauli exclusion. Their values are hard to estimate without the detail knowledge of the potential and wave-functions. Nevertheless, they can be derived from the experiments (Sec. 5.4.2). Once we obtain them, we can solve the above equations for the first order correction $\mu^{(1)}$ and $\Delta_1^{(1)}$. In the above equations, all correction terms either have ζ explicitly or in the similar order. Given the non-singular nature of the crossover problem, we expect the correction $\mu^{(1)}$ and $\Delta_1^{(1)}$ to be also in the order of ζ.

There are three distinct length scales in the problem. The range of the potential, r_c, is the smallest. The intra-channel and inter-channel potentials are essentially zero outside this range. Potential energy dominate kinetic energy in this range and the correlation (wave function) is totally governed by the potential and might have large oscillation. The two-body correlation follows the two-body wave function in this range. The second range is the size of the closed-channel bound-state, a_c. The closed-channel bound state has only negligible weight outside this range. In this range, the many-body correlation still follow the two-body wave function in the closed-channel. We assume that the closed-channel bound state is close to threshold and therefore has most weight in this region. The inter-channel Pauli exclusion are mostly accounted in this region. Not surprisingly, this region contributes most in the integral of λ_1 and λ_2. When much larger than a_c, many-body effects are important. However, the closed-channel has only negligible weight in it and therefore only the open-channel needs to be considered.

Chapter 6

Excitation modes

In the single channel crossover, fermionic modes are related to the two-body correlation of the original fermions; while the bosonic modes are related to the two-body correlation of the auxiliary new bosonic fields (order parameters (Δ_1, Δ_2)). Similarly to the single-channel case, most modes are gapped with minimum at Δ_1 and only one Goldstone mode for the in-phase phase fluctuation of order parameters (bosonic fields) is gapless with linear dispersion at low energy.

6.1 Fermionic excitation modes and Bogoliubov transformation

If we limit ourselves in the mean field level, we can interpret the transformation $T_{\mathbf{k}}L_{\mathbf{k}}$ in Eq. (5.21) as the Bogoliubov canonical transformation, while the 3×3 fermionic correlation matrix B in Eqs. (5.27-5.30) gives us the spectrum of the fermionic quasi-particle excitation. From Eq. (5.14) and Eq. (5.21), the action is diagonal for new fermions (quasi-particles) field

$$\Phi_{\mathbf{k}} \equiv \begin{pmatrix} \phi_{\mathrm{I},+\mathbf{k}} \\ \bar{\phi}_{\mathrm{II},-\mathbf{k}} \\ \bar{\phi}_{\mathrm{III},-\mathbf{k}} \end{pmatrix} = L_{\mathbf{k}}^{\dagger} T_{\mathbf{k}}^{\dagger} \begin{pmatrix} \psi_{a\,\mathbf{k}} \\ \bar{\psi}_{b\,-\mathbf{k}} \\ \bar{\psi}_{c\,-\mathbf{k}} \end{pmatrix}$$

Putting the above transformation into the operator language and using $\mathcal{X}_{\mathrm{I}}$, $\mathcal{X}_{\mathrm{II}}$, and $\mathcal{X}_{\mathrm{III}}$ to denote the new quasi-particles, we have the relation

$$\begin{pmatrix} \mathcal{X}_{\mathrm{I},+\mathbf{k}} \\ \mathcal{X}_{\mathrm{II},-\mathbf{k}}^{\dagger} \\ \mathcal{X}_{\mathrm{III},-\mathbf{k}}^{\dagger} \end{pmatrix} = L_{\mathbf{k}}^{\dagger} T_{\mathbf{k}}^{\dagger} \begin{pmatrix} a_{\mathbf{k}} \\ b_{-\mathbf{k}}^{\dagger} \\ c_{-\mathbf{k}}^{\dagger} \end{pmatrix} \tag{6.1}$$

$$T_k = \begin{pmatrix} u_k & v_k & 0 \\ -v_k & u_k & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{5.22}$$

$$L_{\mathbf{k}} \approx I + \begin{pmatrix} 0 & -\frac{\Delta_1\Delta_2}{4E_{\mathbf{k}}^2} & u_{\mathbf{k}} \\ \frac{\Delta_1\Delta_2}{4E_{\mathbf{k}}^2} & 0 & v_{\mathbf{k}} \\ -u_{\mathbf{k}} & -v_{\mathbf{k}} & 0 \end{pmatrix} \frac{\Delta_2}{\eta} \equiv I + \delta_k \qquad L_{\mathbf{k}}^\dagger = I - \delta_{\mathbf{k}} \tag{5.31}$$

First of all, mixture of $a_{\mathbf{k}}$ and $b_{-\mathbf{k}}^\dagger$ ($c_{-\mathbf{k}}^\dagger$) indicates the pairing of atoms of the opposite momentum. Furthermore, mixture of creators and annihilators dictates the approach of the grand-canonical ensemble, i.e., the ground state is a number non-conserved state. In addition, L matrix cannot be separated into two channels, which indicate the mixture of two channels. At the mean field level, both Δ_1 and Δ_2 are taken as real and constant. The new Hamiltonian at this level is

$$\hat{H} = f(\Delta_1, \Delta_2) + E_{1\,\mathbf{k}} \mathcal{X}_{\mathrm{I},+\mathbf{k}}^\dagger \mathcal{X}_{\mathrm{I},+\mathbf{k}} + E_{2\,\mathbf{k}} \mathcal{X}_{\mathrm{II},-\mathbf{k}}^\dagger \mathcal{X}_{\mathrm{II},-\mathbf{k}} + E_{3\,\mathbf{k}} \mathcal{X}_{\mathrm{III},-\mathbf{k}}^\dagger \mathcal{X}_{\mathrm{III},-\mathbf{k}} \tag{6.2}$$

And the spectrum is just like we calculated in Sec. 5.3, Eqs. 5.28-5.30. We quote here again

$$E_{1\mathbf{k}} \equiv E_{\mathbf{k}} + \gamma_{1\mathbf{k}} \approx E_{\mathbf{k}} + u_{\mathbf{k}}^2 \zeta \tag{5.28}$$

$$E_{2\mathbf{k}} \equiv E_{\mathbf{k}} + \gamma_{2\mathbf{k}} \approx E_{\mathbf{k}} - v_{\mathbf{k}}^2 \zeta \tag{5.29}$$

$$E_{3\mathbf{k}} \equiv \xi_{\mathbf{k}} + \eta + \gamma_{3\mathbf{k}} \approx \epsilon_{\mathbf{k}} + \eta + \frac{\zeta}{2} \tag{5.30}$$

Here γ_1, γ_2 and γ_3 are correction due to the inter-channel Pauli exclusion.

This clearly shows that $\mathcal{X}_{\mathrm{I},\mathbf{k}}^\dagger$, $\mathcal{X}_{\mathrm{II},\mathbf{k}}^\dagger$, and $\mathcal{X}_{\mathrm{III},\mathbf{k}}^\dagger$ are fermionic quasi-particle excitation modes with spectrum $E_{i\,\mathbf{k}}$ and $L_{\mathbf{k}}^\dagger T_{\mathbf{k}}^\dagger$ is the Bogoliubov canonical transformation to transfer the normal fermionic modes into these elementary quasi-particle modes . Here we see in the excitation, different species of opposite momentum, (a, b) and (a, c), mixed together to form the elementary excitation due to the paring in the ground state. From Eqs. (5.28-5.30), we see that the fermionic excitation modes basically follow the pattern in the broad resonance. In the broad resonance where the closed-channel only modifies the interaction in the open-channel, there are three fermionic quasi-particle modes: two (degenerate) Bogoliubov quasi-particle modes in the open-channel, $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_1^2}$ as in BCS theory (gapped at Δ_1 in the BCS-like states, $\mu > 0$ and $\sqrt{\mu^2 + \Delta_1^2}$ in the BEC-like states, $\mu < 0$) ; and one high fermionic excitation mode in the closed-channel, $\xi_{\mathbf{k}} + \eta$, as in normal gas. In the narrow resonance, first of all, the mean-field value of the gap Δ_1 (or

$\sqrt{\mu^2 + \Delta_1^2}$) itself is modified as described in the last chapter (Sec. 5.5). Once that is taken into account, the above conclusion is approximately correct except high-order corrections in ζ. The originally double degenerate excitation modes, $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_1^2}$, now split by $\zeta\Delta_1$; while the third high excitation mode corresponding to the normal fermionic excitation in the closed-channel has a small correction in the same order. On the other respect, as discussed earlier in Sec. 5.3, corrections due to the inter-channel Pauli exclusion do not vanish when the inter-channel coupling, Y, approaches zero.

6.2 Collective excitation modes

Fermionic modes are derived from the correlation function $\hat{\mathcal{G}}^{-1}$ of the fermion fields Ψ, and therefore are mostly single (quasi)particle like. On the other hand, order parameters (Δ_1, Δ_2) are defined in terms of collective behavior of many fermion atoms. Fluctuations of order parameters thus marked the collective excitation modes of the system. Here with a two-component order parameter, four independent modes exist: two for magnitude variation of each Δ_i, internal phase between two Δ_i, and the overall local phase $\theta(x)$ of Δ_1 and Δ_2. The first three change the magnitude of action and therefore massive; while the last one leaves the action invariant and thus massless. We study two modes of the phase fluctuation. The in-phase mode is the counterpart of the Anderson-Bogoliubov modes in the single channel problem; while the two channels introduce a new out-of-phase mode.

For the single-channel crossover, Sec. 4.2 considers all (magnitude and phase) modes of the order parameter fluctuation at the same time, and only calculates the low sound-like part of the spectrum. In the two-channel case, a general analysis with all modes in becomes unwieldy. We instead focus on one mode a time. We isolate the change in one mode and leave others at zero.

6.2.1 The in-phase phase fluctuation

The action of Δ, $S(\bar{\Delta}_i, \Delta_i)$ (Eqs. 5.19, 5.20), is invariant if the phases of $\Delta_{1\,\mathbf{k}}$ and $\Delta_{2\,\mathbf{k}}$ rotate simultaneously. We therefore conclude that there exists a massless (Goldstone) mode corresponding to the local phase invariance. We first study the massless two-channel in-phase phase fluctuation. Introduce the phase fluctuation θ,

$$\Delta_i(x) \to \Delta_i e^{i2\theta(x)} \qquad \bar{\Delta}_i(x) \to \bar{\Delta}_i e^{-i2\theta(x)}$$

This is equivalent to phase rotation of fermionic variable ψ

$$\psi_i(x) \to \psi_i(x) e^{i\theta(x)} \qquad \bar{\psi}_i(x) \to \bar{\psi}_i(x) e^{-i\theta(x)}$$

Again, the phase $\theta(x)$ is common for both channels. With a phase shift, we can rewrite the action (taken mean-field value $\Delta^{(0)} = (\Delta_1, \Delta_2)^\dagger$) (here we follow treatment of Nagaosa [Nagaosa, 1999])

$$S[\theta, \bar{\psi}_i, \psi_i] = S_0[\bar{\psi}_i, \psi_i] + S_1[\theta, \bar{\psi}_i, \psi_i] + S_2[\theta, \bar{\psi}_i, \psi_i] \tag{6.3a}$$

$$S_0[\bar{\psi}_i, \psi_i] = \int dx \Big\{ \sum_j \bar{\psi}_j (\partial_\tau - \frac{1}{2m}\nabla^2 - \mu + \eta_j)\psi_j + \Delta^{(0)\dagger}\tilde{U}^{-1}\Delta^{(0)} - (\bar{\psi}\bar{\psi})\Delta^{(0)} - \Delta^{(0)\dagger}(\psi\psi) \Big\} \tag{6.3b}$$

$$S_1[\theta, \bar{\psi}_i, \psi_i] = \int dx \sum_j \Big\{ i\,\bar{\psi}_j(\partial_\tau\theta)\psi_j + \nabla\theta \cdot \frac{1}{2mi}[\bar{\psi}_j\nabla\psi_j - (\nabla\bar{\psi}_j)\psi_j] \Big\} \tag{6.3c}$$

$$S_2[\theta, \bar{\psi}_i, \psi_i] = \int dx \sum_j \frac{1}{2m}(\nabla\theta)^2\bar{\psi}_j\psi_j \tag{6.3d}$$

Note that here $\Delta^{(0)}$ is the mean-field value of Δ_i, a constant 2-component vector, no longer a functional variable. Here we see that S_0 has the same form as before except it only takes the mean field value of Δ and it is described by the same correlation G_0 (Eq. 5.19). We can regard S_1 and S_2 as perturbation for the so-called gradient expansion on $\nabla\theta$ [Altland and Simons, 2010]. It is then obvious that S_1 is in the first order while S_2 is in the second order regarding with the (time or space) derivative of θ. Use the same spinor representation as before, S is bilinear of ψ and therefore we can formally integrate out ψ.

$$S[\theta] = const. + \ln\det\hat{\mathcal{G}}^{-1}(\theta) \tag{6.4}$$

We write out the formal Green's function according to the above action (with respect to the Nambu-like spinor)

$$\hat{\mathcal{G}}^{-1} = G_0^{-1} + K_1 + K_2, \tag{6.5a}$$

$$K_{1\,k,k'} = \frac{1}{(\beta V)^{1/2}}(\omega_n - \omega_{n'})\theta(k-k')\sigma_3 + \frac{1}{(\beta V)^{1/2}} i\frac{(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{k}+\mathbf{k}')}{2m}\theta(k-k')\hat{1} \tag{6.5b}$$

$$K_{2\,k,k'} = \frac{1}{2m}\sum_{q,q'}\frac{1}{\beta V}(\mathbf{q}\cdot\mathbf{q}')\theta(q)\theta(q')\delta(q+q'+k-k')\sigma_3 \tag{6.5c}$$

where G_0 is the same as (Eqs. 5.17, 5.19). Here $k = (\omega_n, \mathbf{k})$ and $k' = (\omega_{n'}, \mathbf{k}')$. Like in the single channel, $\hat{1}$ is 3×3 identity matrix, and

$$\sigma_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{6.6}$$

As the expansion in Eq. 4.20, we can look for the expansion of $\hat{\mathcal{G}}^{-1}$ over $K_{1,2}$.

$$\mathrm{tr}\ln\hat{\mathcal{G}}^{-1} = \mathrm{tr}\ln{\hat{G}_0}^{-1} + \mathrm{tr}(\hat{G}_0\hat{K}) - \frac{1}{2}\mathrm{tr}(\hat{G}_0\hat{K}\hat{G}_0\hat{K}) + \cdots \tag{4.20}$$

For the first order, $\mathrm{tr}(\hat{G}_0\hat{K})$,

$$\mathrm{tr}(\hat{G}_0\hat{K}_1) = \sum_k G_{0\,k}K_{1\,k,k} = 0 \tag{6.7}$$

$$\begin{aligned}\mathrm{tr}(\hat{G}_0\hat{K}_2) &= \sum_k G_{0\,k}K_{2\,k,k} \\ &= -\frac{1}{2m}\frac{1}{\beta V}\sum_k \mathrm{tr}(\hat{G}_{0\,k}\sigma_3)\sum_q q^2\theta q\theta{-q} \\ &= -\frac{n}{2m}\sum_q q^2\theta(q)\ \theta(-q)\end{aligned} \tag{6.8}$$

Here we use the fact $\frac{1}{\beta V}\sum_k \mathrm{tr}(\hat{G}_{0\,k}\sigma_3) = n$. $\mathrm{tr}(\hat{G}_0\hat{K}_2)$ is already in the second order of θ, and we only need to keep the expansion of K_2 to this order. On the other hand, we have to go to the second order of K_1 for the second order of θ.

$$\mathrm{tr}(\hat{G}_0K_1\hat{G}_0K_1) = \sum_{k,q}\mathrm{tr}(\hat{G}_{0,k+q}K_{1\,k+q,k}\hat{G}_{0\,k}K_{1\,k,k+q}) \tag{6.9}$$

$$\begin{aligned}=&\frac{1}{\beta V}\sum_{k,q=(\omega_m,\mathbf{q})}\theta(q)\theta(-q)\Big[(-\omega_m^2)\mathrm{tr}(\hat{G}_{0,k+q}\sigma_3\hat{G}_{0\,k}\sigma_3) \\ &+\frac{1}{m^2}\sum_{i,j=(x,y,z)} q_iq_j(k_i+\frac{q_i}{2})(k_j+\frac{q_j}{2})\mathrm{tr}(\hat{G}_{0,k+q}\hat{G}_{0\,k})\Big]\end{aligned} \tag{6.10}$$

$$\equiv\sum_q\theta(q)\theta(-q)\big[-\pi^{(0)}(q)\omega_m^2 + \sum_{i,j=(x,y,z)}\pi_{ij}^{(\perp)}(q)q_iq_j\big] \tag{6.11}$$

Here we introduce $q = (\omega_m, \mathbf{q}) = k - k'$. *We can take $q = 0$ in $\pi^{(0)}(q)$ and $\pi^{(\perp)}(q)$ for low frequency and momentum ($\omega_m, \frac{1}{2m}|\mathbf{q}|^2 \ll \Delta_{1,2}$).* Use the previous result of Sec. 5.3, we can calculate the Green's function in the lowest and the first order of ζ in π's. After some long but straightforward algebra (see Appendix. B.4), we find

$$\pi^{(0)}(0) \approx \sum_{\mathbf{k}}\frac{\Delta_1^2}{E_{\mathbf{k}}^3} - \sum_{\mathbf{k}}\frac{\Delta_1^2\Delta_2^2\xi_{\mathbf{k}}}{2E_{\mathbf{k}}^5(\xi_{\mathbf{k}}+\eta)} \tag{6.12}$$

$$\pi^{(\perp)}(0) = 0 \tag{6.13}$$

Combining all these together, we have a new action for the phase fluctuation θ

$$S[\theta] = \int dx \sum_q \theta(q)\theta(-q)\big[\frac{1}{2}\pi^{(0)}(0)\omega_m^2 - \frac{n}{2m}q^2\big] \tag{6.14}$$

The correlation determines the velocity of the Anderson-Bogoliubov collective mode. The second term in Eq. (6.12), $-\sum_{\mathbf{k}} \frac{\Delta_1^2\Delta_2^2\xi_{\mathbf{k}}}{2E_{\mathbf{k}}^5(\xi_{\mathbf{k}}+\eta)} \approx -\sum_{\mathbf{k}} \frac{\Delta_1^3}{2E_{\mathbf{k}}^3}\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\frac{1}{E_{\mathbf{k}}}\zeta$, is the only correction in the next order. Thus, this mode is qualitatively similar as the one in the single-channel with some correction in the order of $\zeta \ll 1$ (see Appendix B.5).

6.2.2 The out-of-phase phase fluctuation

Another interesting phase fluctuation of order parameters is the phase fluctuation in two channels out of sync. This mode is unique for a two-channel system without any counterpart in the single-channel model. When the phase fluctuation of two channels are out of sync, the inter-channel coupling strength changes. Thus, it is expected to be a gapped (massive) mode. We narrow down to the mode that the phases of two atoms (ψ_b and ψ_c) are opposite and leave all other modes constant.

$$\begin{pmatrix}\psi_a(x)\\ \psi_b(x)\\ \psi_c(x)\end{pmatrix} \to \begin{pmatrix}\psi_a(x)\\ \psi_b(x)e^{+i\theta(x)}\\ \psi_c(x)e^{-i\theta(x)}\end{pmatrix} \qquad \begin{pmatrix}\bar{\psi}_a(x)\\ \bar{\psi}_b(x)\\ \bar{\psi}_c(x)\end{pmatrix} \to \begin{pmatrix}\bar{\psi}_a(x)\\ \bar{\psi}_b(x)e^{-i\theta(x)}\\ \bar{\psi}_c(x)e^{+i\theta(x)}\end{pmatrix}$$

The order parameters do not have a simple transformation because they are connected to two channels via 2×2 interaction matrix $\tilde{U}$, which mixes two channels (Eq. 5.11).

$$\begin{pmatrix}\Delta_1(x)\\ \Delta_2(x)\end{pmatrix} \to \begin{pmatrix}U & Y\\ Y^* & V\end{pmatrix}\begin{pmatrix}\psi_b\psi_a(x)e^{+i\theta(x)}\\ \psi_c\psi_a(x)e^{-i\theta(x)}\end{pmatrix}$$

This term cannot be easily written in terms of mean-field value Δ_i. On the other hand, as mentioned before, we freeze all other modes to their mean-field value except θ. We therefore use another two-component of atom pairs$(\psi_b\psi_a, \psi_c\psi_a)$, which is the linear recombination of (Δ_1, Δ_2).

Comparing to the in-phase phase rotation, the out-of-phase one does modify the action's magnitude.

Write the interaction term in the momentum space,

$$\begin{aligned}
&\Delta^\dagger \tilde{U}^{-1}\Delta \\
=&\begin{pmatrix} \langle\bar{\psi}_b\bar{\psi}_a\rangle e^{-i\theta} & \langle\bar{\psi}_c\bar{\psi}_a\rangle e^{+i\theta}\end{pmatrix}\tilde{U}\tilde{U}^{-1}\tilde{U}\begin{pmatrix}\langle\psi_b\psi_a\rangle e^{+i\theta}\\ \langle\psi_c\psi_a\rangle e^{-i\theta}\end{pmatrix}\\
=&\begin{pmatrix}\tilde{h}_1^* & \tilde{h}_2^*\end{pmatrix}\begin{pmatrix}U & Ye^{-i2\theta}\\ Y^*e^{+i2\theta} & V\end{pmatrix}\begin{pmatrix}\tilde{h}_1\\ \tilde{h}_2\end{pmatrix}\\
=&\Delta^{(0)\dagger}\tilde{U}^{-1}\Delta^{(0)}+\left[Y(e^{-i2\theta}-1)\tilde{h}_1^*\tilde{h}_2+Y^*(e^{+i2\theta}-1)\tilde{h}_1\tilde{h}_2^*\right]
\end{aligned}$$

Note that here we take the mean-field expectation of pairs of fermions $\tilde{h}_1 = \langle\psi_b\psi_a\rangle = \sum_{\mathbf{k}} h_{1\mathbf{k}}$, $\tilde{h}_2 = \langle\psi_c\psi_a\rangle = \sum_{\mathbf{k}} h_{2\mathbf{k}}$, and their complex conjugates[1]. Comparing with the action of the in-phase phase fluctuation (Eq. 6.3), we find one more terms in the new action.

$$\begin{aligned}
S[\theta,\bar{\psi}_i,\psi_i] =& S_0[\bar{\psi}_i,\psi_i]+S_1[\theta,\bar{\psi}_i,\psi_i]+S_2[\theta,\bar{\psi}_i,\psi_i]+S_3[\theta] && \text{(6.15a)}\\
S_0[\bar{\psi}_i,\psi_i] =& \int dx\Big\{\sum_{j=(a,b,c)}\bar{\psi}_j(\partial_\tau-\frac{1}{2m}\nabla^2-\mu+\eta_j)\psi_j\\
&+\Delta^{(0)\dagger}\tilde{U}^{-1}\Delta^{(0)}-(\bar{\psi}\bar{\psi})\Delta^{(0)}-\Delta^{(0)\dagger}(\psi\psi)\Big\} && \text{(6.15b)}\\
S_1[\theta,\bar{\psi}_i,\psi_i] =& \int dx\Big\{i\,(\partial_\tau\theta)(\bar{\psi}_b\psi_b-\bar{\psi}_c\psi_c) && \text{(6.15c)}\\
&+\nabla\theta\cdot\frac{1}{2mi}[\bar{\psi}_b\nabla\psi_b-\bar{\psi}_c\nabla\psi_c-(\nabla\bar{\psi}_b)\psi_b+(\nabla\bar{\psi}_c)\psi_c]\Big\} && \text{(6.15d)}\\
S_2[\theta,\bar{\psi}_i,\psi_i] =& \int dx\frac{1}{2m}(\nabla\theta)^2(\bar{\psi}_b\psi_b+\bar{\psi}_c\psi_c) && \text{(6.15e)}\\
S_3[\theta] =& \int dx\left[Y(e^{-i2\theta}-1)\tilde{h}_1^*\tilde{h}_2+Y^*(e^{+i2\theta}-1)\tilde{h}_1\tilde{h}_2^*\right] && \text{(6.15f)}
\end{aligned}$$

Let us look at S_3 first. We can expand it around small θ.

$$\begin{aligned}
S_3[\theta] =& \int dx\left[Y(e^{-i2\theta}-1)\tilde{h}_1^*\tilde{h}_2+Y^*(e^{+i2\theta}-1)\tilde{h}_1\tilde{h}_2^*\right] && \text{(6.16)}\\
=& \int dx-i2\left[Y\tilde{h}_1^*\tilde{h}_2-Y^*\tilde{h}_1\tilde{h}_2^*\right]\theta-2\left[Y\tilde{h}_1^*\tilde{h}_2+Y^*\tilde{h}_1\tilde{h}_2^*\right]\theta^2 && \text{(6.17)}
\end{aligned}$$

From Eq. 5.37

$$h_{1\mathbf{k}} = \Delta_1\frac{E_{1\,\mathbf{k}}+\xi_{\mathbf{k}}+\eta}{(E_{1\,\mathbf{k}}+E_{2\,\mathbf{k}})(E_{1\,\mathbf{k}}+E_{3\,\mathbf{k}})}$$

If $\Delta_1\to\Delta_1 e^{i\varphi}$, all $h_{1\mathbf{k}}$ has argument φ (or $\pi+\varphi$). Thus $\tilde{h}_1$ has argument φ (or $\pi+\varphi$) as well. Also consider

[1] $\psi\psi$ and $\bar{\psi}\bar{\psi}$ are complex conjugate in the mean-field level.

the mean-field equation $\Delta_1 = U\tilde{h}_1 + Y\tilde{h}_2$, We can rewrite

$$Y\tilde{h}_1^*\tilde{h}_2 = \tilde{h}_1^*\Delta_1 - \tilde{h}_1^*U\tilde{h}_1 \tag{6.18}$$

U is real for a Hermite interaction. So this quantity is real. In addition, $Y^*\tilde{h}_1\tilde{h}_2^*$ is complex conjugate of $Y\tilde{h}_2\tilde{h}_1^*$. So they are equal because they are both real. From all these, we conclude that the linear term of θ vanishes. This is actually expected for a perturbation around the saddle point. Now we can rewrite this term

$$S_3[\theta] = \int dx - 4Y\tilde{h}_1^*\tilde{h}_2\theta^2 = \sum_q \theta(q)\theta(-q)(-4Y\tilde{h}_1^*\tilde{h}_2) \tag{6.19}$$

$Y\tilde{h}_1^*\tilde{h}_2$ is actually the expectation of coupling for the two channel correlation. It is not hard to see that this value is negative in the minimum (saddle point).

The other two terms in the expansion of the action, S_1 and S_2, go in the same way as the in-phase phase fluctuation except an extra $\frac{1}{2}$ because only hyperfine species (b and c) participates. They actually produce the same result except only a half of the particles (b, c) participates. $(n_b + n_c = n_a = n/2)$ The full action about θ is

$$S[\theta] = \int dx \sum_q \theta(q)\theta(-q)\big[\frac{1}{4}\pi^{(0)}(0)(\omega_m^2 - \omega_0^2) - \frac{n}{4m}q^2\big] \tag{6.20}$$

where

$$\omega_0^2 = -\frac{16Y\tilde{h}_1^*\tilde{h}_2}{\pi^{(0)}(0)} \tag{6.21}$$

As expected, the out-of-phase phase mode is a gapped mode, with a spectrum starting from ω_0. When two channels' phases fluctuate out-of-phase, the original self-consistent mean-field equation cannot be satisfied and this fluctuation is coupled with the fermionic modes. Its general spectrum is expected to related to the pair-breaking energy, but Eq. 6.20 can only be calculated numerically in general. Particularly, $Y\tilde{h}_1^*\tilde{h}_2$ is hard to estimate except at the ends of crossover. At the BCS end, $Y\tilde{h}_1^*\tilde{h}_2$ is close the expectation of the interaction energy calculated according to the effective interaction in the open-channel. We can estimate it as $Y\tilde{h}_1^*\tilde{h}_2 \sim -N(0)\Delta_1^2$, where $N(0)$ is the density of the state at the Fermi energy. $\pi^{(0)}(0) \sim N(0)$. So we can estimate that $\omega_0 \sim \Delta_1$. This mode is inside the fermionic excitation spectrum. At the BEC end, the interaction energy in the open-channel can be estimated roughly as $N_{\text{open}}|\mu|$; $\pi^{(0)}(0) \sim \mathcal{V}_0\Delta_1^2/|\mu|^{3/2}$. Note that here the open-channel atom number N_{open} might be significantly smaller than the total atom number. Here, $\Delta_1 \sim n_o^{1/2}a_s^{-1/2}$ and $|\mu| \sim a_s^{-2}$. Put all these together, $\omega_0 \sim n^{1/2}|\mu|^{5/4}/\Delta_1 \sim a_s^{-2}$. It is in the order of the ionization (pair breaking) energy again and is only related to two-body physics.

Chapter 7

Conclusions

In this thesis, we study the narrow Feshbach resonance in the three-species case where two channels share the same species.

In general, for the narrow resonance without a shared species, the main correction to the single-channel result comes from the extra counting of the atoms in the open-channel, which leads to the extra shift 2μ in $\tilde{a}_s$, and the closed-channel, which leads to the extra number equation. Two number equations exist, one for the open-channel and one for the closed-channel. The open-channel number equation resembles the number equation of the single-channel model.

When there is a common species, however, the Pauli exclusion between two channels due to the common species in the three-species narrow resonance, calls for careful consideration. Our treatment follows the spirit of the so-called "universality" idea. For a dilute system with a short-range potential, such as the dilute ultracold alkali gas, the short-range part of a two-body correlation does not significantly change from two-body to many-body. This particular feature justifies using the two-body quantities (e.g. the s-wave scattering length a_s) as the boundary condition for the many-body correlations. The most part of the correlations, where no two particles are close in short-range, is essentially free from interaction. This long-range part of the correlations does change from two-body to many-body. Unique in our problem is the involvement of the Feshbach resonance. A resonance makes the system extremely sensitive to even small change in the relative weight between two channels. We use the fact that, in the Feshbach resonance, the closed-channel bound state, ϕ_0, as a short-range object, is still not very sensitive to the resonance; hence, we can, within the universality idea, apply a simple boundary condition to the closed-channel correlation. However, the indirect interaction mediated by the closed-channel dominates the direct interaction within the open-channel. Consequently, a small change in the closed-channel bound-state weight *does* affect the short-range wave function in the open-channel, originally expressed through the boundary condition using the s-wave scattering length a_s.

When the spatial extension of the closed-channel bound state is of the order of the inter-particle distance, a_0, or even larger, the Feshbach resonance in the many-body context is a genuine three-species many-body

problem and no simple solution is available. By contrast, when the bound-state's spatial extension is much smaller than the interparticle distance, the ratio (a_c/a_0) serves as the expansion parameter and we can extract the effect of the inter-channel Pauli exclusion perturbatively. In essence, we can then ignore the many-body effects within closed-channel bound-states, while only taking into consideration the Pauli exclusion between channels. A few new parameters need to be introduced and can be calibrated from experiments, such as λ_1 (Eq. 5.48), λ_2 (Eq. 5.49). Mean field properties can still be determined through gap equations and number equations similar as in the single-channel case. The excitation modes are also close to the original single-channel result with correction of the order of a_c/a_0, where a_c is the spatial extension of the uncoupled closed-channel bound state and a_0 is the average interparticle distance.

We can distinguish three different regimes for the many-body energy scale E_F when compared with the two-body physics.

1. The regime where E_F is much smaller than the characteristic energy δ_c (See Eq. 3.19 in Sec. 3). Around resonance, the closed-channel weight is negligible in this regime. We can then ignore the closed-channel completely and approximate the effective open-channel interaction by a pseudo-potential characterized by the s-wave scattering length, a_s.

2. The regime where E_F is larger than δ_c, but smaller than the closed-channel bound state binding energy E_b, or the bare detuning η. The closed-channel weight is significant in this regime and cannot be ignored, which means $n_{\text{open}} + n_{\text{close}} = n_{\text{total}}$. Also, we need to take into account the fact that, in the resonance formula of a_s, shifting should be counted from the Fermi surface instead of from zero as in two-body physics. These effects, considered previously [Gurarie and Radzihovsky, 2007], are also carefully analyzed in this thesis. Furthermore, the Pauli exclusion between two channels needs to be taken into account when these two channels share a common species. Nevertheless, at low momentum, where the open-channel has most of its weight, the closed-channel bound state only has very small weight. Consequently, we can still treat the Pauli exclusion between channels perturbatively using the expansion coefficient E_F/η.

3. The regime where E_F is larger than the binding energy E_b or the bare detuning η. We have a genuine three-species many-body problem. This regime can be achieved in two ways. One way requires a very large E_F, which indicates a very dense system. However, it would be hard to imagine that the original dilute alkali gas model still applies in this case. Various approximations in the model would probably break down beforehand, such as the pseudo-potential approximation with a_s. The second way requires a very small η, which indicates a genuine three-species many-body problem. This remains an open

problem.

This thesis focuses on the second regime. Careful analysis leads us to distinguish two related but different concepts, the total weight of the closed-channel and the weight of the closed-channel in a particular momentum level. Within our assumptions, namely, the spatial extension of a closed-channel bound state is much smaller than the interparticle distance, a very low occupation in low-momentum levels ($k \lesssim k_F$) of the closed-channel persists despite the large total weight of the closed-channel. A suitable small parameter E_F/η (or a_0/a_c), upon which a perturbation theory can be developed over a non-perturbative zeroth order solution, emerges with this discovery. Pairing in many-body problems is known to be non-perturbative and has to be handled with proper non-perturbative techniques. Nonetheless, we can concentrate the non-perturbative part into the zeroth order (broad resonance) solution, while treating the other corrections perturbatively. The resulting theory handles the two channels in steps self-consistently[1].

In summary, a two-channel model has a two-component order parameter (Δ_1, Δ_2): one component for each channel. The order parameter for the closed-channel can be determined by the number equation of the closed-channel (Eq. 5.61)

$$N_{close} \approx \sum_{\mathbf{k}} \frac{\Delta_2^2}{(\xi_{\mathbf{k}} + \eta)(2\xi_{\mathbf{k}} + \eta)} \tag{5.61}$$

Where $\xi_{\mathbf{k}} = \hbar^2 k^2/2m - \mu$ and η is the energy difference between two channels. The renormalized gap equation is given in Eq. 5.53

$$1 = \frac{4\pi \tilde{a}_s(\mu, \lambda_1)}{m} \sum \left(\frac{1}{2E_{\mathbf{k}}} - \frac{1}{2\epsilon_{\mathbf{k}}} - \frac{\Delta_2^2 \xi_{\mathbf{k}}}{4(\xi_{\mathbf{k}} + \eta)E_{\mathbf{k}}^3}\right) - \frac{\lambda_2}{\Delta_1} \tag{5.53}$$

where $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_1^2}$. Here, $\tilde{a}_s(\mu, \lambda_1)$ is the two-body open-channel effective s-wave scattering length with an additional shifting $2\mu + \lambda_1$ as Eq. 5.50.

$$a_s = a_{\rm bg}\left(1 + \frac{\mathcal{K}}{\delta - 2\mu - \lambda_1}\right) \tag{5.50}$$

λ_1 and λ_2 are two new parameters describing the overlapping of the two channels, and they can be calibrated from experiments (see Eqs. 5.48 5.49, and Sec. 5.4.2). The open-channel number equation is Eq. 5.62

$$N_{open} \approx \sum_{\mathbf{k}} \left[\frac{E_{\mathbf{k}} - \xi_{\mathbf{k}}}{2E_{\mathbf{k}}}\left(1 + \frac{\Delta_1}{\eta}\zeta\right) - \frac{\Delta_1^3}{4E_{\mathbf{k}}^3}\zeta\right] \tag{5.62}$$

Here $\zeta = \Delta_2^2/\Delta_1\eta \ll E_{\mathbf{k}}$ appears in multiple places as the small expansion parameter. The open-channel

[1]Here by "self-consistent", we refer to the self-consistency in treating the close-channel according to zeroth order in the open-channel pairing. The BCS-type treatment of pairing in the open-channel is known to be not self-consistent.

number equation and the associated gap equation need to be solved self-consistently to get the mean field result (Δ_1 and μ). One of the most noteworthy new phenomena is probably that the open-channel gap Δ_1 saturates in the BEC side of a narrow resonance.

There are three fermionic excitation modes. Their spectrums with the first order correction due to the inter-channel Pauli exclusion are given by Eqs. 5.28-5.30

$$E_{1\mathbf{k}} \approx E_{\mathbf{k}} + u_{\mathbf{k}}^2 \Delta_1 \zeta \tag{5.28}$$

$$E_{2\mathbf{k}} \approx E_{\mathbf{k}} - v_{\mathbf{k}}^2 \Delta_1 \zeta \tag{5.29}$$

$$E_{3\mathbf{k}} \approx \epsilon_{\mathbf{k}} + \eta + \frac{\zeta}{2} \Delta_1 \tag{5.30}$$

With a two-component order parameter, the bosonic collective fluctuation modes are rich. We explored two modes about phase fluctuations. The two-component in-phase fluctuation is massless and the low-energy one. It is similar to the Anderson-Bogoliubov modes in the single-channel problem with a small correction in the order of ζ. The new out-of-phase fluctuation is gapped and the minimum excitation energy is in the order of the pair-breaking energy (Δ_1 in the BCS-like states, $\mu > 0$ and $\sqrt{\mu^2 + \Delta_1^2}$ in the BEC-like states, $\mu < 0$).

In our approach, we take the broad resonance result (or the single-channel crossover) as our zeroth order solution, upon which the expansion is performed. It is however known that the simple BCS-type pairing treatment is not adequate to quantitatively describe the whole BEC-BCS crossover region. Therefore the zeroth order solution used in this thesis (simple BCS type ansatz or saddle point) can be improved through further theoretical development. Nevertheless, we expect the perturbative approach used here to build the narrow resonance from the single-channel crossover result to be still valid then. Once the zeroth order solution (for a broad resonance or a single channel BEC-BCS crossover model) is patched over with whatever advancement, the correction of the narrow resonance in such a parameter regime, can still be obtained with a procedure similar as the one discussed in this thesis.

The theory we have developed here is for zero-temperature only. This limit simplifies the calculations considerably. However, an extension to finite temperature along the same spirit should be possible. The two-component order parameters should persist at low-temperature. At higher temperature, these components are likely to decay at different temperatures. The open-channel order parameter, associated with a much lower energy scale (of the order of the Fermi energy or even lower), should turn to zero first. Then the system becomes a normal gas with a Feshbach resonance. From the above discussion, many-body corrections due to the narrow resonance (both the intra- and inter-channel Pauli exclusion) seem to be agnostic to whether

the system is in superfluid state or not. Thus, we expect that these many-body corrections can be carried out in a similar fashion. There should still be corrections over the detuning due to the chemical potential and the inter-channel Pauli exclusion (λ_1) although a system is more likely to be a Fermi liquid in the BCS side and a gas of normal fermion-dimer-molecules on the BEC side in such a temperature.

Appendix A

The variational approach using the BCS-type ansatz

We can also formulate the problem using the BCS-type ansatz. It is not difficult to calculate the expectation of the free energy as well as the wave function that optimizes the free energy within this ansatz. The optimization process gives us gap equations, which determine the wave function with the constraint from number equations. We will see that this method yields the mean-field solution consistent with the one of the path-integral approach. However, this method is mean-field by nature and difficult to be extended for studying collective excitations.

We rewrite the Hamiltonian Eq. 5.6 in momentum space, and restore the momentum dependence of the interaction coefficients.

$$\begin{aligned} H = & \sum_{\mathbf{k}} \epsilon^a_{\mathbf{k}} a^+_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon^b_{\mathbf{k}} b^+_{\mathbf{k}} b_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon^c_{\mathbf{k}} c^+_{\mathbf{k}} c_{\mathbf{k}} \\ & - \sum_{\mathbf{k}\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} a^+_{\mathbf{k}} b^+_{-\mathbf{k}} b_{-\mathbf{k}'} a_{\mathbf{k}'} - \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} a^+_{\mathbf{k}} c^+_{-\mathbf{k}} c_{-\mathbf{k}'} a_{\mathbf{k}'} \\ & - \sum_{\mathbf{k}\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} a^+_{\mathbf{k}} b^+_{-\mathbf{k}} c_{-\mathbf{k}'} a_{\mathbf{k}'} - \sum_{\mathbf{k}\mathbf{k}'} Y^*_{\mathbf{k}\mathbf{k}'} a^+_{\mathbf{k}'} c^+_{-\mathbf{k}'} b_{-\mathbf{k}} a_{\mathbf{k}} \end{aligned} \tag{A.1}$$

Here we only keep the zero center-of-mass momentum paring terms as in the original BCS work [Bardeen et al., 1957]. We take the free atom at zero magnetic field as the zero energy.

$$\epsilon^i_{\mathbf{k}} = k^2/(2m) + \eta^i, \qquad (i = a, b, c)$$

η^i is the Zeeman energy of the i^{th} atom at magnetic field B. The hermiticity of the Hamiltonian imposes

$$U_{\mathbf{k}'\mathbf{k}} = U^*_{\mathbf{k}\mathbf{k}'}, \qquad V_{\mathbf{k}'\mathbf{k}} = V^*_{\mathbf{k}\mathbf{k}'} \tag{A.2}$$

We then introduce the BCS-type ansatz

$$|\Psi\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} + w_{\mathbf{k}} a^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}} \right) |0\rangle \tag{A.3}$$

$|0\rangle$ is the particle vacuum state. We require $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 + |w_{\mathbf{k}}|^2 = 1$ for normalization. This ansatz is constructed like the original BCS ansatz for superconductivity. An alternative ansatz would be $\prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}})(u'_{\mathbf{k}} + w_{\mathbf{k}} a^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}})\,|0\rangle$, which is actually the same as Eq. A.3, because the cross term vanishes due to the Pauli exclusion on the common species. As the original BCS ansatz, this ansatz does not have the fixed particle number. We will just require the expected value of number operators match the total particle number. For all interaction terms, we get two types of contributions, for example,

$$\left\langle U_{\mathbf{k}\mathbf{k}'} a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} b_{-\mathbf{k}'} a_{\mathbf{k}'} \right\rangle = \sum_{\mathbf{k}} U_{\mathbf{k}\mathbf{k}} |v_{\mathbf{k}}|^2 + \sum_{\mathbf{k}\neq\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} v_{\mathbf{k}'} u^*_{\mathbf{k}'} u_{\mathbf{k}} v^*_{\mathbf{k}}$$

The first term is the Hatree term and the second term is the more interesting pairing term.

This gives the full free energy as

$$\begin{aligned}
&F \equiv \left\langle H - \mu N \right\rangle \\
=&\sum (\xi^a_{\mathbf{k}} + \xi^b_{\mathbf{k}})\,|v_{\mathbf{k}}|^2 + \sum (\xi^a_{\mathbf{k}} + \xi^c_{\mathbf{k}})\,|w_{\mathbf{k}}|^2 \\
&- \sum_{\mathbf{k}} U_{\mathbf{k}\mathbf{k}} |v_{\mathbf{k}}|^2 - \sum_{\mathbf{k}\neq\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} v_{\mathbf{k}'} u^*_{\mathbf{k}'} u_{\mathbf{k}} v^*_{\mathbf{k}} \\
&- \sum_{\mathbf{k}} V_{\mathbf{k}\mathbf{k}} |w_{\mathbf{k}}|^2 - \sum_{\mathbf{k}\neq\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} w_{\mathbf{k}'} u^*_{\mathbf{k}'} u_{\mathbf{k}} w^*_{\mathbf{k}} \\
&- \sum_{\mathbf{k}} Y_{\mathbf{k}\mathbf{k}} w_{\mathbf{k}} v^*_{\mathbf{k}} - \sum_{\mathbf{k}\neq\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} w_{\mathbf{k}'} u^*_{\mathbf{k}'} v^*_{\mathbf{k}} u_{\mathbf{k}} \\
&- \sum_{\mathbf{k}} Y^*_{\mathbf{k}\mathbf{k}} w^*_{\mathbf{k}} v_{\mathbf{k}} - \sum_{\mathbf{k}\neq\mathbf{k}'} Y^*_{\mathbf{k}\mathbf{k}'} w^*_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}'} u^*_{\mathbf{k}'}
\end{aligned} \tag{A.4}$$

where we have set

$$\xi^a_{\mathbf{k}} = \epsilon^a_{\mathbf{k}} - \mu^a, \qquad \xi^b_{\mathbf{k}} = \epsilon^b_{\mathbf{k}} - \mu^b, \qquad \xi^c_{\mathbf{k}} = \epsilon^c_{\mathbf{k}} - \mu^b$$

Two chemical potentials are added to make sure the $n_a = n_b + n_c = \frac{1}{2}n$. In principle, μ^a does not need to be equal to μ^b as there is no exchange or conversion between (a) and (b, c). In fact, the structure of the ansatz guarantees that $n_a = n_b + n_c$. Therefore, we set $\mu^a = \mu^b$ for simplicity and drop the superscript on chemical potential hereinafter. We will also drop the Hartree terms because they are only related to the density and thus can be absorbed into the chemical potentials. In the second summation, we will ignore the fact that the summation only goes through $\mathbf{k} \neq \mathbf{k}'$ because the corrections due to this restriction lead to only the higher order terms.

A.1 Exact gap equations and number equations

We introduce two new parameters $h_{1\mathbf{k}}$ and $h_{2\mathbf{k}}$, which corresponds to the mean field values (equal time average) of the anomalous Green's functions, (in the same way as $h_{1,2}$ in Sec 5.4),

$$u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 + w_{\mathbf{k}}^2 = 1 \tag{A.5}$$

$$u_{\mathbf{k}} v_{\mathbf{k}} = h_{1\mathbf{k}} \tag{A.6}$$

$$u_{\mathbf{k}} w_{\mathbf{k}} = h_{2\mathbf{k}} \tag{A.7}$$

We can solve $u_{\mathbf{k}}$, $v_{\mathbf{k}}$, $w_{\mathbf{k}}$ in terms of $h_{1\mathbf{k}}$ and $h_{2\mathbf{k}}$ (all parameters are taken as real)[1]. One complication in solving above equations is that $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ and $w_{\mathbf{k}}$ are all monotonic functions of $\mathbf{k}$, while $h_{1\mathbf{k}}$ or $h_{2\mathbf{k}}$ is not in the BCS end. So, we need to be careful when taking the square root. We introduce sgn_k for such purpose.

$$\begin{aligned}
u_{\mathbf{k}}^2 =& \frac{1}{2}\left(1 + \mathrm{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}\right) \\
v_{\mathbf{k}}^2 =& \frac{2h_{1\mathbf{k}}^2}{1 + \mathrm{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}} = \frac{h_{1\mathbf{k}}^2}{2(h_{1\mathbf{k}}^2 + h_{2\mathbf{k}}^2)}\left(1 - \mathrm{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}\right) \\
w_{\mathbf{k}}^2 =& \frac{2h_{2\mathbf{k}}^2}{1 + \mathrm{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}} = \frac{h_{2\mathbf{k}}^2}{2(h_{1\mathbf{k}}^2 + h_{2\mathbf{k}}^2)}\left(1 - \mathrm{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}\right)
\end{aligned} \tag{A.8}$$

where $\mathrm{sgn}_k = 1$ for all k in BEC cases, and for large k in BCS cases. In BCS cases, $\mathrm{sgn}_k = -1$ when k is small. In the single-channel crossover, $\mathrm{sgn}_k = \mathrm{sgn}(\epsilon_k - \mu)$, and the turning point is at $u_{\mathbf{k}}^2 = 1/2$ which corresponds to zero chemical potential, $\mu = 0$. The two-channel crossover is more delicate to treat. The turning point is still at $u_{\mathbf{k}}^2 = 1/2$, but it is no longer exactly at $\mu = 0$. The sgn_k function is very important in number equations Eqs. A.14. They however can be absorbed later on, after we convert the formulas back into notations of ($u_{\mathbf{k}}$, $v_{\mathbf{k}}$, $w_{\mathbf{k}}$) or ξ_k.

[1] It is not hard to prove that the parameters that optimize the free energy are real, within an overall phase factor, when the interactions are real. (See also footnote 5 in Chapter 5, page 39.)

Eq. A.8's derivatives over $h_{1\mathbf{k}}$ are[2]

$$\begin{aligned}
\frac{\partial u_{\mathbf{k}}^2}{\partial h_{1\mathbf{k}}} =& -\frac{2h_{1\mathbf{k}}}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}}\mathrm{sgn}_k \\
\frac{\partial v_{\mathbf{k}}^2}{\partial h_{1\mathbf{k}}} =& \frac{2h_{1\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}} - \frac{8h_{1\mathbf{k}}h_{2\mathbf{k}}^2\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\left(1+\mathrm{sgn}_k\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\right)^2} \\
\frac{\partial w_{\mathbf{k}}^2}{\partial h_{1\mathbf{k}}} =& \frac{8h_{1\mathbf{k}}h_{2\mathbf{k}}^2\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\left(1+\mathrm{sgn}_k\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\right)^2} \\
=& \mathrm{sgn}_k\frac{h_{1\mathbf{k}}h_{2\mathbf{k}}^2\left(1-\mathrm{sgn}_k\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\right)^2}{2\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}(h_{1\mathbf{k}}^2+h_{2\mathbf{k}}^2)^2}
\end{aligned} \tag{A.9}$$

The second equation is not very obvious, but can be obtained by noting that $\frac{\partial v_{\mathbf{k}}^2}{\partial h_{1\mathbf{k}}} = -\frac{\partial u_{\mathbf{k}}^2}{\partial h_{1\mathbf{k}}} - \frac{\partial w_{\mathbf{k}}^2}{\partial h_{1\mathbf{k}}}$. Similarly, derivatives over $h_{2\mathbf{k}}$ are

$$\begin{aligned}
\frac{\partial u_{\mathbf{k}}^2}{\partial h_{2\mathbf{k}}} =& -\frac{2h_{2\mathbf{k}}}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}}\mathrm{sgn}_k \\
\frac{\partial v_{\mathbf{k}}^2}{\partial h_{2\mathbf{k}}} =& \frac{8h_{1\mathbf{k}}^2h_{2\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\left(1+\mathrm{sgn}_k\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\right)^2} \\
=& \mathrm{sgn}_k\frac{h_{1\mathbf{k}}^2h_{2\mathbf{k}}\left(1-\mathrm{sgn}_k\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\right)^2}{2\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}(h_{1\mathbf{k}}^2+h_{2\mathbf{k}}^2)^2} \\
\frac{\partial w_{\mathbf{k}}^2}{\partial h_{2\mathbf{k}}} =& \frac{2h_{2\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}} - \frac{8h_{1\mathbf{k}}^2h_{2\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\left(1+\mathrm{sgn}_k\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\right)^2}
\end{aligned} \tag{A.10}$$

We can obtain the gap equations by differentiating the free energy with respect to $h_{1\mathbf{k}}$ and $h_{2\mathbf{k}}$.

$$\begin{aligned}
&\frac{h_{1\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}}\xi_{\mathbf{k}}^{ab} + \frac{4h_{1\mathbf{k}}h_{2\mathbf{k}}^2\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\left(1+\mathrm{sgn}_k\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\right)^2}\eta \\
&\qquad - \sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'}h_{1\mathbf{k}'} - \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'}h_{2\mathbf{k}'} = 0
\end{aligned} \tag{A.11a}$$

$$\begin{aligned}
&\frac{h_{2\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}}\xi_{\mathbf{k}}^{ac} - \frac{4h_{1\mathbf{k}}^2h_{2\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\left(1+\mathrm{sgn}_k\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\right)^2}\eta \\
&\qquad - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}h_{2\mathbf{k}'} - \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'}h_{1\mathbf{k}'} = 0
\end{aligned} \tag{A.11b}$$

where $\eta = \epsilon_{\mathbf{k}}^{ac} - \epsilon_{\mathbf{k}}^{ab} = \eta^c - \eta^b$ is the bare Zeeman energy difference and is larger than most other energy scales,

[2]Here we follow the same convention by taking $h_{1\mathbf{k}}$ and $h_{2\mathbf{k}}$ as real

such as E_F. It is close to the binding energy of the closed-channel bound state when it is not too far away from the resonance point. We see one disadvantages of the ansatz method: unlike the path integral approach, where $h_{1\mathbf{k}}$ and $h_{2\mathbf{k}}$ have a very specific forms, Eqs. (5.37, 5.38), and ready for further approximation and analysis, we do not have much guide for these two quantities here and need to make some guess.

We can define order parameters

$$\Delta_{1\mathbf{k}} = \sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'} + \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} h_{2\mathbf{k}'} \tag{A.12}$$

$$\Delta_{2\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} h_{2\mathbf{k}'} + \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'} \tag{A.13}$$

Both of them should have little $\mathbf{k}$-dependence at low momentum for short-range interactions. We will drop the $\mathbf{k}$ subscripts in both Δ in the following. Two number equations can be obtained. One for each channel.

$$N_{\text{open}} = 2\sum_{\mathbf{k}} v_{\mathbf{k}}^2 = \sum_{\mathbf{k}} \frac{h_{1\mathbf{k}}^2}{(h_{1\mathbf{k}}^2 + h_{2\mathbf{k}}^2)} \left(1 - \text{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}\right) \tag{A.14a}$$

$$N_{\text{close}} = 2\sum_{\mathbf{k}} w_{\mathbf{k}}^2 = \sum_{\mathbf{k}} \frac{h_{2\mathbf{k}}^2}{(h_{1\mathbf{k}}^2 + h_{2\mathbf{k}}^2)} \left(1 - \text{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}\right) \tag{A.14b}$$

A.2 Approximate solution of the mean field equations

Here instead of solving these equations, we just demonstrate that they are consistent to the saddle point solution obtained in the path-integral method up to the first order of correction ζ.

Let us look at the closed-channel gap equation (Eq. A.11b) first. It can be rewritten as

$$\frac{h_{2\mathbf{k}}\text{sgn}_k}{\sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}} \left(2\xi_{\mathbf{k}} + \eta - \frac{4h_{1\mathbf{k}}^2}{\left(1 + \text{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}\right)^2} \eta\right) - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} h_{2\mathbf{k}'} - \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'} = 0$$

We can put some terms back into the notation of ($u_{\mathbf{k}}$, $v_{\mathbf{k}}$, $w_{\mathbf{k}}$).

$$\text{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2} = (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 - w_{\mathbf{k}}^2) \tag{A.15}$$

$$1 + \text{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2} = 2u_{\mathbf{k}}^2 \tag{A.16}$$

$$\frac{4h_{1\mathbf{k}}^2}{\left(1 + \text{sgn}_k \sqrt{1 - 4h_{1\mathbf{k}}^2 - 4h_{2\mathbf{k}}^2}\right)^2} = \frac{v_{\mathbf{k}}^2}{u_{\mathbf{k}}^2} \tag{A.17}$$

We rewrite the closed-channel gap equation using these relations

$$\frac{h_{2\mathbf{k}}}{u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 - w_{\mathbf{k}}^2}\left(2\xi_{\mathbf{k}} + \eta - \frac{v_{\mathbf{k}}^2}{u_{\mathbf{k}}^2}\eta\right) - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} h_{2\mathbf{k}'} - \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'} = 0$$

At high momentum ($\gg k_F$), the third term in the parenthesis is negligible and the the denominator $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 - w_{\mathbf{k}}^2 \approx 1$. This equation is then very similar to the two-body Schrödinger equation (Eq. 3.4). For the closed-channel, the interaction, or the closed-channel bound state, ϕ_0, has non-zero value for a range in the momentum space much larger than k_F. Thus we expect the closed-channel correlation $h_{2\mathbf{k}} \propto \phi_0 f(\mathbf{k})$ where $f(\mathbf{k})$ approach one at high momentum. This is in fact the same argument as Eq. 5.1 in the beginning of Chapter 5. The next thing to notice is that the third term in the parenthesis might dominate the other two terms in certain situation (low momentum, BCS) because the denominator $u_{\mathbf{k}}^2$ can be very small in such regions. A nature way to compensate this big term is to set[3] $f(\mathbf{k}) = u_{\mathbf{k}}^2$. Now we arrive the same conclusion for the closed-channel correlation as in the path-integral approach (Eq. 5.42)

$$h_{2\mathbf{k}} = \tilde{\alpha}\phi_{0\mathbf{k}} u_{\mathbf{k}}^2 \tag{A.18}$$

Note that $\tilde{\alpha}$ is not fixed yet and should not be identified as α in the path-integral approach (Eq. 5.42) *a prior*. The equation becomes,

$$\frac{\tilde{\alpha}\phi_{0\mathbf{k}} u_{\mathbf{k}}^2}{u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 - w_{\mathbf{k}}^2}\left(2\xi_{\mathbf{k}} + \eta - \frac{v_{\mathbf{k}}^2}{u_{\mathbf{k}}^2}\eta\right) - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\tilde{\alpha}\phi_{0\mathbf{k}} u_{\mathbf{k}}^2 - \sum_{\mathbf{k}'} Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'} = 0$$

Using the similar approach as in the path-integral method, we multiply the equation with $\phi_{0\mathbf{k}}^*$ and integrate the equation in order to find $\tilde{\alpha}$. In the denominator of the first term $u_{\mathbf{k}}^2 \gg v_{\mathbf{k}}^2$, $u_{\mathbf{k}}^2 \gg w_{\mathbf{k}}^2$ in the most of the integral domains (up to order of $\kappa(\eta)$ in the momentum space). The equation is approximately

$$\tilde{\alpha}\sum_{\mathbf{k}} \frac{\phi_{0\mathbf{k}}\phi_{0\mathbf{k}}^* u_{\mathbf{k}}^2}{u_{\mathbf{k}}^2}\left(2\xi_{\mathbf{k}} + \eta\right) - \tilde{\alpha}\sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\phi_{0\mathbf{k}}\phi_{0\mathbf{k}}^* u_{\mathbf{k}}^2 - \sum_{\mathbf{k}\mathbf{k}'} \phi_{0\mathbf{k}}^* Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'} = 0$$

And it is not hard to find

$$\tilde{\alpha} \approx \frac{\sum_{\mathbf{k}\mathbf{k}'} \phi_{\mathbf{k}}^* Y_{\mathbf{k}\mathbf{k}'} h_{1\mathbf{k}'}}{-E_b + \eta - 2\mu - \tilde{\lambda}_1} \tag{A.19}$$

And $\tilde{\lambda}_1$ is simpler than Eq. 5.48

$$\tilde{\lambda}_1(\eta) \equiv -\sum_{\mathbf{k}\mathbf{k}'} \phi_{\mathbf{k}}^* v_{\mathbf{k}'}^2 V_{\mathbf{k}\mathbf{k}'}\phi_{\mathbf{k}'}$$

[3] $u_{\mathbf{k}}^2$ in Chapter 5 is defined to be $(\xi_{\mathbf{k}} + E_{\mathbf{k}})/2E_{\mathbf{k}}$ and does not carry an obvious physical meaning as $u_{\mathbf{k}}^2$ in this appendix. They are the same in the lowest order of our expansion over ζ for the narrow resonance. This does not affect our analysis because the closed-channel correlation is actually a first order quantity.

But it should be equal to λ_1 from the path-integral approach at the first order of ζ (Eq. 5.48) because this term is the dominated one (see Sec. 5.4.2, Eq. 5.55). We will just use λ_1 hereinafter. $\tilde{\alpha}$ is the same as α in the path-integral approach if $h_{1\mathbf{k}}$ here is the same as the one in the path-integral approach, which we will show in the following. Particularly for low momentum, $\phi_{0\mathbf{k}} \sim \frac{1}{\eta+\epsilon_{\mathbf{k}}}$ (see Appendix B.3) and it is not hard to find at low momentum

$$\alpha\phi_{0\mathbf{k}} \overset{k\lesssim k_F}{=} \frac{\Delta_2}{\eta} \tag{A.20}$$

Now let us check the open-channel gap equation. We can rewrite it as

$$\frac{h_{1\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}}\left(\xi_{\mathbf{k}}^{ab}+\frac{4h_{2\mathbf{k}}^2}{\left(1+\mathrm{sgn}_k\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}\right)^2}\eta\right)=\Delta_1$$

Again, using Eq. A.16, we replace the denominator with $2u_{\mathbf{k}}^2$. Also we replace $h_{2\mathbf{k}}$ with $\tilde{\alpha}\phi_{0\mathbf{k}}u_{\mathbf{k}}^2$ using Eq. A.18.

$$\frac{h_{1\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}}\left(2\xi_{\mathbf{k}}+(\tilde{\alpha}\phi_{0\mathbf{k}})^2\eta\right)=\Delta_1$$

At low momentum, the second term in the parenthesis can be simplified as $\Delta_2^2/\eta=\zeta\Delta_1$ using Eq. A.20

$$\frac{h_{1\mathbf{k}}\mathrm{sgn}_k}{\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2}}\left(2\xi_{\mathbf{k}}+\zeta\Delta_1\right)=\Delta_1$$

We can solve $h_{1\mathbf{k}}$ in terms of Δ_1.

$$h_{1\mathbf{k}}^2=\frac{\Delta_1^2(1-4h_{2\mathbf{k}}^2)}{(2\xi_{\mathbf{k}}+\zeta\Delta_1)^2+4\Delta_1^2}\approx\frac{\Delta_1^2(1-4h_{2\mathbf{k}}^2)}{4E_{\mathbf{k}}^2+4\xi_{\mathbf{k}}\Delta_1\zeta}\approx\frac{\Delta_1^2}{4E_{\mathbf{k}}^2}(1-\frac{\xi_{\mathbf{k}}\Delta_1}{E_{\mathbf{k}}^2}\zeta)(1-4\frac{\Delta_1}{\eta}u_{\mathbf{k}}^4\zeta)$$

Here we take the low momentum value of $h_{2\mathbf{k}}^2\approx\frac{\Delta_1}{\eta}u_{\mathbf{k}}^4\zeta$ in the last step. This term is much smaller than $\frac{\xi_{\mathbf{k}}\zeta}{E_{\mathbf{k}}^2}$ because of the factor $\frac{\Delta_1}{\eta}$ at the low momentum. We can neglect this term. Now we have

$$h_{1\mathbf{k}}^2\approx\frac{\Delta_1^2}{4E_{\mathbf{k}}^2}(1-\frac{\xi_{\mathbf{k}}\Delta_1}{E_{\mathbf{k}}^2}\zeta) \tag{A.21}$$

This is equivalent in the first order of ζ to the $h_{1\mathbf{k}}$ in the path-integral approach (Eq. 5.37).

It is easy to see that $h_{2\mathbf{k}}^2$ is the higher order as ζ and $w_{\mathbf{k}}\ll 1$ all the time. So we always have $h_{2\mathbf{k}}\approx w_{\mathbf{k}}$ except in low momentum. However, the summation in the low momentum is very small, one order higher in ζ. The closed-channel number equation is then simply $N_{\mathrm{closed}}=\sum w_{\mathbf{k}}^2\approx\sum_{\mathbf{k}}h_{2\mathbf{k}}^2$, which is the same result in the path-integral approach as we discussed in Eq. 5.61.

We move to the open-channel number equation Eq. A.14a. At the momentum smaller than the charac-

teristic momentum of the closed-channel bound state κ ($\eta \sim E_b = \kappa^2/2m$), factor $\frac{h_{1\mathbf{k}}^2}{(h_{1\mathbf{k}}^2+h_{2\mathbf{k}}^2)}$ is approximately 1,

$$\frac{h_{1\mathbf{k}}^2}{(h_{1\mathbf{k}}^2+h_{2\mathbf{k}}^2)} = 1 - \frac{h_{2\mathbf{k}}^2}{(h_{1\mathbf{k}}^2+h_{2\mathbf{k}}^2)} \overset{k\ll\kappa}{\approx} 1 - \frac{h_{2\mathbf{k}}^2}{h_{1\mathbf{k}}^2} \approx 1 - \frac{4E_{\mathbf{k}}^2}{\eta\Delta_1} u_{\mathbf{k}^4}\zeta \sim 1 + O(\zeta^2)$$

while on the high momentum

$$\frac{h_{1\mathbf{k}}^2}{(h_{1\mathbf{k}}^2+h_{2\mathbf{k}}^2)} \overset{k\gtrsim\kappa}{\approx} \frac{\frac{\Delta_1^2}{4E_{\mathbf{k}}^2}}{\frac{\Delta_2^2}{\eta+\epsilon_{\mathbf{k}}}} \sim \frac{\Delta_1^2}{\epsilon_{\mathbf{k}}\Delta_2} \ll 1$$

Therefore the factor $\frac{h_{1\mathbf{k}}^2}{(h_{1\mathbf{k}}^2+h_{2\mathbf{k}}^2)}$ limit the summation into low momentum. On the other hand, in the low momentum we have, $\frac{h_{2\mathbf{k}}^2}{h_{1\mathbf{k}}^2} \sim \frac{\Delta_1}{\eta}\zeta$, thus we can neglect $h_{2\mathbf{k}}^2$ in the square root comparing to $h_{1\mathbf{k}}^2$. And using Eq. A.21

$$\sqrt{1-4h_{1\mathbf{k}}^2-4h_{2\mathbf{k}}^2} \approx \sqrt{1-4h_{1\mathbf{k}}^2+O(\zeta^2)} \approx \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} + \frac{\Delta_1^2}{4E_{\mathbf{k}}^3}\zeta + O(\zeta^2)$$

So we have the open-channel number equation

$$N_{\text{open}} \approx \sum_{\mathbf{k}} 1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} - \frac{\Delta_1^3}{4E_{\mathbf{k}}^3}\zeta \tag{A.22}$$

This is consistent to the open-channel number equation derived from the path-integral approach (Eq. 5.62, where the second term is negligible comparing to the third term).

Thus we have shown that the mean-field solution of the path-integral approach can solve the gap equations and number equations of the ansatz method up to the first order of ζ.

Appendix B

Materials for Chapter 5

B.1 Diagonalization of the matrix Eq. (5.25)

We need to find a unitary transformation L to diagonalize the matrix

$$T_k^\dagger G^{-1}_{\omega_n,\mathbf{k}} T_k = i\omega_n I + \begin{pmatrix} -E_k & 0 & u_k\Delta_2 \\ 0 & +E_k & v_k\Delta_2 \\ u_k\Delta_2 & v_k\Delta_2 & +\xi_k+\eta \end{pmatrix} \tag{5.25}$$

We drops all the k subscripts in this section because matrices in this section are decoupled in momentum and we only deal with one particular momentum $\mathbf{k}$ a time. We notice that the first term is proportional to an identity matrix and does not change by unitary transformation, we only need to concentrate on the second term. We rescale all elements with $E_\mathbf{k}$ for simplicity in the following of this section.

$$y = \frac{\Delta_2}{E_\mathbf{k}}, \qquad t = \frac{\xi_k+\eta}{E_\mathbf{k}},$$

$$R = \begin{pmatrix} -1 & 0 & uy \\ 0 & 1 & vy \\ uy & vy & t \end{pmatrix}$$

The secular equation of R is ($|x\,I - R| = 0$)

$$(x^2-1)(x-t) - y^2 x + (u^2-v^2)y^2 = 0 \tag{B.1}$$

We use $u^2+v^2=1$ here. We assume at the zeroth order, the three eigenvalues are -1, 1 and t. (t has weak dependency on energy as $(\xi_k+\eta)/E_k$, however, at the low energy region of interest, we ignore ξ_k.) Both y and t are larger than 1, however, we will verify that given condition $y^2 \ll t$, the correction is indeed

small and the expansion is reasonable (See Sec.B.5). *Indeed, close-channel component can still be smaller than the open-channel component at low-k (in the order of k_F) due to the close-channel bound state is much smaller than the interparticle distance even when the total close-channel atom number is more than that of open-channel. And here all the quantities are about low-k unless specifically noticed.* We expand the system to the first order of the dimensionless parameter $\tilde{\zeta} = y^2/t$ (Eq. 5.26), and find

$$\begin{array}{ccc} x^{(0)} & x^{(1)} & Eigenvector \\ -1 & -u^2\tilde{\zeta} & \left(1 \quad \frac{uvy^2}{2t} \quad -\frac{uy}{t}\right) \\ 1 & -v^2\tilde{\zeta} & \left(-\frac{uvy^2}{2t} \quad 1 \quad -\frac{vy}{t}\right) \\ t & \frac{1}{2}\tilde{\zeta} & \left(\frac{uy}{t} \quad \frac{vy}{t} \quad 1\right) \end{array}$$

Now it is easy to write down the corresponding diagonal matrix and the unitary transformation

$$B = i\omega_n I + E \begin{pmatrix} -1-u^2\tilde{\zeta} & 0 & 0 \\ 0 & 1-v^2\tilde{\zeta} & 0 \\ 0 & 0 & t\frac{1}{2}\tilde{\zeta} \end{pmatrix} \tag{B.2}$$

$$L = \begin{pmatrix} 1 & -\frac{uvy^2}{2t} & \frac{uy}{t} \\ \frac{uvy^2}{2t} & 1 & \frac{vy}{t} \\ -\frac{uy}{t} & -\frac{vy}{t} & 1 \end{pmatrix} \tag{B.3}$$

Here L is not exactly unitary transformation, it is only unitary in the first order of $\tilde{\zeta}$. We have

$$B = i\omega_n I + E\, L^\dagger R L + o(\tilde{\zeta})$$

Alternatively, we can write L as

$$L = I + \begin{pmatrix} 0 & -\frac{\Delta_1\Delta_2}{4E^2} & u \\ \frac{\Delta_1\Delta_2}{4E^2} & 0 & v \\ -u & v & 0 \end{pmatrix} \frac{\Delta_2}{\eta} \tag{B.4}$$

Here we use $uv = \Delta_1/2E$.

In the above treatment, the small parameter $\tilde{\zeta}$ is momentum dependent. If we restore the subscript $\mathbf{k}$

and scale it back with $E_{\mathbf{k}}$

$$\tilde{\zeta} = \frac{\Delta_2^2}{E_{\mathbf{k}}(\xi_{\mathbf{k}} + \eta)} \tag{B.5}$$

A momentum-dependent small parameter is not very convenient to work with, so we take its maximum value in low momentum ($\lesssim E_F$). In the BCS-like states ($\mu > 0$), $\min E_k = \Delta_1$, $\min \xi_{\mathbf{k}} = 0$; in the BEC-like states ($\mu < 0$), $\min E_k = \sqrt{\Delta_1^2 + \mu^2}$ and $\min \xi_{\mathbf{k}} = |\mu|$. We take the smaller values and have our expanding small parameter ζ(Eq. 5.26)

$$\zeta = \max \tilde{\zeta} = \frac{\Delta_2^2}{\Delta_1 \eta} \tag{B.6}$$

B.2 Derivation of the mean-field equations (5.36)

We have fermion correlation as a 3×3 matrix (Eq. 5.19),

$$\mathcal{G}^{-1} = \begin{pmatrix} i\omega_n - \xi_k & \Delta_1 & \Delta_2 \\ \bar{\Delta}_1 & i\omega_n + \xi_k & 0 \\ \bar{\Delta}_2 & 0 & i\omega_n + \xi_k + \eta \end{pmatrix} \tag{5.19}$$

Here we work in the momentum space, in which the system is nicely decoupled at least to the mean-field order. And we therefore drop all the k subscript in the rest of section. A general 3×3 matrix inverted as such,

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{12}^* & A_{22} & 0 \\ A_{13}^* & 0 & A_{33} \end{pmatrix}^{-1} = \frac{1}{|A|} \begin{pmatrix} A_{22}A_{33} & -A_{12}A_{33} & -A_{13}A_{22} \\ -A_{12}^*A_{33} & A_{11}A_{33} - A_{13}A_{13}^* & A_{12}^*A_{13} \\ -A_{13}^*A_{22} & A_{12}A_{13}^* & A_{11}A_{22} - A_{12}A_{12}^* \end{pmatrix} \tag{B.7}$$

where $|A|$ is the determent of A. At the mean field level, all Δ_i's are real constants. We denote the mean field value of $\mathcal{G}$ as G_0. The determent of G_0^{-1} can be expressed as

$$|G_0^{-1}| = (i\omega_n - E_1)(i\omega_n + E_2)(i\omega_n + E_3) \tag{B.8}$$

where E_i's are defined in Eqs. (5.28-5.30). And G_0 can be obtained according to the above rule. Now we can find the last term in 5.34,

$$\begin{aligned}\mathrm{tr}\left[G_0 \cdot \left(\begin{smallmatrix}0&1&0\\0&0&0\\0&0&0\end{smallmatrix}\right)\right] &= \sum_{\mathbf{k}\omega_n} G_{0\,(21)} \\ &= \sum_{\mathbf{k}} \sum_{\omega_n} \frac{-\Delta_1^*(i\omega_n + \xi + \eta)}{(i\omega_n - E_1)(i\omega_n + E_2)(i\omega_n + E_3)} \\ &= \sum_{\mathbf{k}} \Delta_1^* \frac{E_1 + \xi + \eta}{(E_1 + E_2)(E_1 + E_3)} \equiv \sum_{\mathbf{k}} h_{1\,\mathbf{k}}\end{aligned} \tag{B.9}$$

Here we perform the zero-temperature Matsubara summation in the third equal sign with the normal trick (see sec. 4.2.1 in [Altland and Simons, 2010], sec. 25 in [Fetter and Walecka, 1971], also refer to Footnote 2 at Page. 23). Because of zero-temperature, within three roots, E_1, $-E_2$ and $-E_3$, we only need to take into account two negative roots $-E_2$ and $-E_3$, assuming the correction is small. Similarly

$$\mathrm{tr}\left[G_0 \cdot \left(\begin{smallmatrix}0&0&1\\0&0&0\\0&0&0\end{smallmatrix}\right)\right] = \sum_{\mathbf{k}\omega_n} G_{0\,(31)} = \sum_{\mathbf{k}} \Delta_2 \frac{E_1 + \xi}{(E_1 + E_2)(E_1 + E_3)} \equiv \sum_{\mathbf{k}} h_{2\,\mathbf{k}} \tag{B.10}$$

And we have

$$\begin{aligned}(\tilde{U}^{-1})_{11}\bar{\Delta}_1 + (\tilde{U}^{-1})_{21}\bar{\Delta}_2 - \sum_{\mathbf{k}} h_{1\,\mathbf{k}} = 0 \\ (\tilde{U}^{-1})_{12}\bar{\Delta}_1 + (\tilde{U}^{-1})_{22}\bar{\Delta}_2 - \sum_{\mathbf{k}} h_{2\,\mathbf{k}} = 0\end{aligned}$$

Invert the interaction matrix $\tilde{U}$ and we have Eq. 5.36.

B.3 The wave function for a short-range potential

Here we discuss some possible generalization on the wave function for a short-range potential. This topic has been studied by Zhang [Zhang and Leggett, 2009]. We will use some similar ideas. Outside the range r_c of a short-range potential, an atom is free and the Schrödinger equation is very simple.

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \tag{B.11}$$

The equation has a simple solution for s-wave, $\psi = A'e^{-\kappa r}/r$ (κ is imaginary for a scattering state). For a bound state. normalization A' is determined by connecting it with the short-range part of the wave function, φ_0, and then requiring the full wave function normalized to 1.

Let us discuss the bound-state first, where $\kappa > 0$. In the momentum space, there is also a universal behavior at low momentum, where $kr_c \ll 1$.

$$\psi_k = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{r}(\varphi_0 + A' \frac{e^{-\kappa r}}{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$$

The first part for φ_0 corresponds to the short-range part of the wave-function.

$$\psi_k = \varphi_{0\,k} + \frac{1}{(2\pi)^{3/2}} \int d\mathbf{r}(A' \frac{e^{-\kappa r}}{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} = \varphi_{0\,k} - A\frac{1}{k^2+\kappa^2}$$

The first term has very little k dependence for low memontum $k \ll 1/r_c$ and the second terms is more important in this range. Furthermore, if the bound-state is close to threshold, the most weight is outside r_c, we can neglect the first term and we have universal behavior at low-momentum while the normalization factor A can be easily determined.

$$A = \sqrt{\frac{8\pi\kappa}{\mathcal{V}_0}} \tag{B.12}$$

Where $\mathcal{V}_0$ is the total volume of the system. And the wave-function is

$$\psi_{\mathbf{k}} \approx \sqrt{\frac{8\pi\kappa}{\mathcal{V}_0}} \frac{1}{k^2+\kappa^2} \approx \sqrt{\frac{8\pi\kappa}{\mathcal{V}_0}} \frac{1}{\kappa^2} \tag{B.13}$$

The second approximation is when the momentum is low ($\lesssim k_F$).

Besides the bound-state, if the interaction is weak and short-range, the low energy scattering state is well described by the s-wave scattering state $\psi \propto 1/r - 1/a$ (Eq. 2.4), and its Fourier transformation in the momentum space has the similar form $1/k^2$. When considering many-body physics, in the low momentum below or around the Fermi momentum, wave function is modified by the many-body effect; but in the medium momentum, (still much smaller than $1/r_c$), this $1/k^2$ universal behavior is preserved. The distribution of particle in such momentum, $k_F \ll k \ll 1/r_c$, is $1/k^4$. This is actually the "high-momentum" (medium here) behavior (C/k^4) described in Tan's work about universality [Tan, 2008a, Tan, 2008b].

On the other hand, at very higher momentum ($k \gg 1/r_c$), the second term in the above is very small. This is because the smooth tail part of the wave function (ϕ_0) cancels out and contributes little in high frequency momentum oscillation. The high-frequency Fourier component in momentum space is solely determined by the wave function within the potential range (r_c). This can be extend beyond the two-body wave function to the two-body correlation as long as the long-wave-length part is smooth. In all cases, two-body, or many-body, very high-frequency of two-body correlation follows the two-body wave function.

Incidentally, the two-body Schrödinger equation in the momentum space reads as

$$\frac{\hbar^2 k^2}{2m}\psi_{\mathbf{k}} + \sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'}\psi_{\mathbf{k}'} = E\psi_{\mathbf{k}} \tag{B.14}$$

At very high momentum (determined by the interaction strength and potential range), the first term dominates, and we have the asymptotic form of the wave-function similar as Eq. B.13,

$$\lim_{k\to\infty} \psi_{\mathbf{k}} = \tilde{A}\frac{1}{k^2+\kappa^2} \tag{B.15}$$

where $-\frac{\hbar^2\kappa^2}{2m} = E$. Note that this behavior is for a different reason and $\tilde{A}$ is not necessarily equal A at low momentum discussed before.

B.4 Evaluation of $\pi^{(0)}(0)$ and $\pi^{\perp}(0)$

Here we calculate $\pi^{(0)}$ and $\pi^{\perp}$ (Eqs. 6.10, 6.11) to the first order of ζ (Eq. 5.26) using the expansion of the Green's function (Eqs. 5.33) described in Sec. 5.3.

$$\begin{aligned}
\pi^{(0)}(0) &= \sum_k \mathrm{tr}(\hat{G}_{0\,k}\sigma_3\hat{G}_{0\,k}\sigma_3) \\
&\approx \sum_k \mathrm{tr}\big(T_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3\big) \\
&\quad + \mathrm{tr}\Big(T_{\mathbf{k}}\delta_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 - T_{\mathbf{k}}B_k^{-1}\delta_{\mathbf{k}}T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 \\
&\quad + T_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}}\delta_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 - T_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}}B_k^{-1}\delta_{\mathbf{k}}T_{\mathbf{k}}^{\dagger}\sigma_3\Big)
\end{aligned} \tag{B.16}$$

Note that k stands for both the momentum and the Matsubara frequency, $(\omega_n, \mathbf{k})$. $\delta_{\mathbf{k}}$ is defined in Eq. 5.31.

$$\delta_c \equiv \begin{pmatrix} 0 & -\frac{\Delta_1\Delta_2}{4E_{\mathbf{k}}^2} & u_{\mathbf{k}} \\ \frac{\Delta_1\Delta_2}{4E_{\mathbf{k}}^2} & 0 & v_{\mathbf{k}} \\ -u_{\mathbf{k}} & -v_{\mathbf{k}} & 0 \end{pmatrix}\frac{\Delta_2}{\eta}$$

Introduce two matricies M_k and $\widetilde{M}_k$,

$$M_k \equiv T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}}B_k^{-1} \tag{B.17}$$

$$\widetilde{M}_k \equiv B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}}B_k^{-1}T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}} \tag{B.18}$$

And we can rewrite $\pi^{(0)}(0)$ as

$$\pi^{(0)}(0) = \sum_k \mathrm{tr}\big(M_k\big) + 2\mathrm{tr}\Big(\delta_{\mathbf{k}}\widetilde{M_k} - \delta_{\mathbf{k}} M_k\Big) \tag{B.19}$$

Here we use the cyclical property of the trace $\mathrm{tr}(AB) = \mathrm{tr}(BA)$. It is straightforward to calculate

$$T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}} B_k^{-1} = \begin{pmatrix} \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}(i\omega_k - E_{1\,\mathbf{k}})} & \frac{\Delta_1}{E_{\mathbf{k}}(i\omega_k + E_{2\,\mathbf{k}})} & 0 \\ \frac{\Delta_1}{E_{\mathbf{k}}(i\omega_k - E_{1\,\mathbf{k}})} & -\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}(i\omega_k + E_{2\,\mathbf{k}})} & 0 \\ 0 & 0 & -\frac{1}{i\omega_k + E_{3\,\mathbf{k}}} \end{pmatrix}$$

Now it is easy to calculate the first term

$$\sum_k \mathrm{tr}\big(M_k\big) = \sum_k \left[\frac{2\Delta_1^2}{E_{\mathbf{k}}^2(i\omega_k - E_{1\,\mathbf{k}})(i\omega_k + E_{2\,\mathbf{k}})} + \left(\frac{\xi_{\mathbf{k}}^2}{E_{\mathbf{k}}^2(i\omega_k - E_{1\,\mathbf{k}})^2} + \frac{\xi_{\mathbf{k}}^2}{E_{\mathbf{k}}^2(i\omega_k + E_{1\,\mathbf{k}})^2} - \frac{1}{(i\omega_k + E_{3\,\mathbf{k}})^2}\right)\right] \tag{B.20}$$

Only root $-E_{2\,\mathbf{k}}$ in the first term contributes in the Matsubara frequency summation at zero temperature.

$$\sum_k \mathrm{tr}\big(M_k\big) = \sum_{\mathbf{k}} \frac{2\Delta_1^2}{E_{\mathbf{k}}^2(E_{1\,\mathbf{k}} + E_{2\,\mathbf{k}})} \approx \sum_{\mathbf{k}} \frac{\Delta_1^2}{E_{\mathbf{k}}^3} - \sum_{\mathbf{k}} \frac{\Delta_1^2\Delta_2^2\xi_{\mathbf{k}}}{2E_{\mathbf{k}}^5(\xi_{\mathbf{k}} + \eta)} \tag{B.21}$$

For the lowest order of the second term in Eq. (B.16), we only need to take the lowest order of B_k

$$B_k = \begin{pmatrix} i\omega_k - E_{\mathbf{k}} & 0 & 0 \\ 0 & i\omega_k + E_{\mathbf{k}} & 0 \\ 0 & 0 & i\omega_k + \xi_{\mathbf{k}} + \eta \end{pmatrix} \tag{B.22}$$

It is easy to verify at this approximation

$$\mathrm{tr}\Big(\delta_{\mathbf{k}}\widetilde{M_k} - \delta_{\mathbf{k}} M_k\Big) = 0 \tag{B.23}$$

Combine Eq. (B.21) and Eq. (B.23), we have

$$\pi^{(0)}(0) \approx \sum_{\mathbf{k}} \frac{\Delta_1^2}{E_{\mathbf{k}}^3} - \sum_{\mathbf{k}} \frac{\Delta_1^2\Delta_2^2\xi_{\mathbf{k}}}{2E_{\mathbf{k}}^5(\xi_{\mathbf{k}} + \eta)} \tag{B.24}$$

$\pi^{\perp}(0)$ can actually be calculated exactly

$$\pi_{ij}^{\perp}(0) = \sum_{k}(k_i)(k_j)\mathrm{tr}(\hat{G}_{0\,k}\hat{G}_{0\,k}) \tag{B.25}$$

$$\begin{aligned}\mathrm{tr}(\hat{G}_{0\,k}\hat{G}_{0\,k}) =& \sum_{k}\mathrm{tr}\big(T_{\mathbf{k}}L_{\mathbf{k}}B_k^{-1}L_{\mathbf{k}}^{\dagger}T_{\mathbf{k}}^{\dagger}T_{\mathbf{k}}L_{\mathbf{k}}B_k^{-1}L_{\mathbf{k}}^{\dagger}T_{\mathbf{k}}^{\dagger}\big)\\ =& \sum_{k}\mathrm{tr}\big(B_k^{-1}B_k^{-1}\big)\\ =& \sum_{\mathbf{k},i}(\sum_{\omega_n}(i\omega_k-\xi_i)^{-2})\\ =& 0\end{aligned} \tag{B.26}$$

B.5 Consistency of the expansion over ζ

In our treatment here, one crucial assumption in expansion is the smallness of Δ_2/η comparing to 1. Here we check it. We have the closed-channel gap equation (Eq. 5.40)

$$\Delta_2 = \sum Y h_{1\mathbf{k}} + \sum V h_{2\mathbf{k}} \tag{5.40}$$

The first term on the right is relatively small comparing to the second term. We just keep the second term for estimation. Furthermore, we assume $h_{2\,\mathbf{k}} = \sqrt{N_c}\phi_{0\,\mathbf{k}}$, where $\phi_{0\,\mathbf{k}}$ is the normalized wave function of the isolated closed-channel potential satisfying Schrödinger equation (Eq. 5.43)

$$-E_b^{(0)}\phi_{0\,\mathbf{p}} = 2\epsilon_{\mathbf{p}}\phi_{0\,\mathbf{p}} - \sum_{\mathbf{k}} V\phi_{0\,\mathbf{k}} \tag{5.43}$$

Rearranging it, we have (especially at low momentum)

$$\sum_{\mathbf{k}} V\phi_{0\,\mathbf{k}} = (2\epsilon_{\mathbf{p}} + E_b)\phi_{0\,\mathbf{p}} \approx \eta\phi_{0\,\mathbf{p}}$$

Here E_b is the binding energy of the closed-channel bound state and η is the Zeeman energy difference. The second approximation is correct at low momentum (smaller or in the same order of the Fermi momentum) as $\epsilon_{\mathbf{p}} \ll E_b \approx \eta$ not too far away from the resonance. Put all these together, we have

$$\Delta_2 \approx \alpha E_b \phi_{k=0}$$

If we assume a simple exponentially decayed wave function as in Eq. B.13 from Sec. B.3

$$\phi_{\mathbf{k}} = \sqrt{\frac{8\pi\kappa}{\mathcal{V}_0}} \frac{1}{k^2+\kappa^2} \approx \sqrt{\frac{8\pi\kappa}{\mathcal{V}_0}} \frac{1}{\kappa^2} \tag{B.13}$$

Here $\mathcal{V}_0$ is the total volume and κ is the characteristic momentum of the closed-channel bound state, $\eta \approx E_b = \hbar^2\kappa^2/2m$. The second approximation above is only for low momentum. Collect all these together, we have

$$\Delta_2 \approx \sqrt{N_c}\eta\sqrt{\frac{8\pi\kappa}{\mathcal{V}_0}} \frac{1}{\kappa^2} \sim \eta\sqrt{\frac{n_c}{\kappa^3}} \sim \eta \left(\frac{k_{Fc}}{\kappa}\right)^{\frac{3}{2}} \sim \eta \left(\frac{E_{Fc}}{\eta}\right)^{\frac{3}{4}} \tag{B.27}$$

k_{Fc} is the Fermi momentum corresponding to density of atoms in the close-channel, which is much smaller than the characteristic momentum for the bound-state, κ. Therefore we have $\Delta_2 \ll \eta$, even when n_c is close to the total density n.

Now we check whether the corrections in Fermionic spectrum (Eqs. 5.28-5.30), are indeed small comparing to the zeroth order terms.

$$E_{1\mathbf{k}} \approx E_{\mathbf{k}} + u_{\mathbf{k}}^2\Delta_1\zeta \tag{5.28}$$

$$E_{2\mathbf{k}} \approx E_{\mathbf{k}} - v_{\mathbf{k}}^2\Delta_1\zeta \tag{5.29}$$

$$E_{3\mathbf{k}} \approx \epsilon_{\mathbf{k}} + \eta + \frac{\zeta}{2}\Delta_1 \tag{5.30}$$

Here, we mostly only concern of case of low momentum ($k \sim k_F$). In Eq. 5.30,

$$\frac{\zeta\Delta_1}{E_{3\mathbf{k}}} \sim \frac{\Delta_2^2}{\eta^2} \sim \left(\frac{k_{Fc}}{\kappa}\right)^3 \ll 1$$

Eq. 5.28 and Eq. 5.29 are slightly more complicated. Both of them involve $\frac{\Delta_2^2}{E_{\mathbf{k}}\eta}$, at the BCS limit, the closed-channel density is small, $k_{F\,c}$ is small and that makes this ratio small; when close to the (narrow) resonance, where n_c is comparable to to the total density, at low energy, Δ_1 is in the order of the Fermi energy, so does $E_{\mathbf{k}}$. We have (we no longer distinguish $k_{F\,c}$ with k_F)

$$\zeta = \frac{\Delta_2^2}{\Delta_1\eta} \sim \frac{\eta^2\frac{k_{Fc}^3}{\kappa^3}}{k_F^2\eta} \sim \frac{k_F}{\kappa} \ll 1 \tag{B.28}$$

More deeply, in the secular equation that leads to spectrum, Eq. B.1. We rewrite it without scaling to $E_{\mathbf{k}}$, (We drop subscript $\mathbf{k}$ in the following equations for simplicity)

$$(x^2-E^2)(x-\xi-\eta) - \Delta_2^2 x + \Delta_2^2 E(u^2-v^2) = 0$$

It is not hard to use definition of u and v to find $u^2 - v^2 = \xi/E$, and express $E^2 = \xi^2 + \Delta_1^2$. Therefore we have

$$(x-\xi)(x+\xi)(x-\xi-\eta) - \Delta_1^2(x-\xi-\eta) - \Delta_2^2(x-\xi) = 0$$

Here the first term is for free particles, and let us estimate the relative size of the last two terms. For low-momentum solution, we simply use $\Delta_1 \sim E_F$, we find

$$\frac{\Delta_1^2(x-\xi-\eta)}{\Delta_2^2(x-\xi)} \sim \frac{E_F^2\eta}{\Delta_2^2 E_F} \sim \frac{\kappa}{k_F} \gg 1$$

This justifies our choice to neglect the last term when finding the lowest-order solution and then use the last term for correction.

In another word, the above estimation is just saying that the total occupation number of the closed-channel at a low momentum level is much smaller than 1 in all regions of resonance (narrow or broad) because the closed-channel bound state is much smaller than the interparticle distance. This factor gives us a small factor, $\zeta \sim \frac{r_c}{a_0} \sim \frac{k_F}{\kappa} \sim \sqrt{\frac{E_F}{\eta}}$, upon which we can do the expansion.

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