THEORY OF BCS-BEC CROSSOVER IN ULTRA-COLD ATOMIC GASES

by

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Abstract

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In ultracold atomic fermions, the sign and the magnitude of pairing interactions can be controlled by using the magnetically-tuned Feshbach resonances to achieve a continuos transition between Cooper pairs of dilute fermi gas to BEC of diatomic molecules, which is known as the “BCS-BEC crossover”. At present, although several models have been proposed, there is still no exact analytical solution of the many-body problem of BCS-BEC crossover region. The standard BCS mean field theory of superconductivity was used [1–3] to describe the whole crossover resulting a useful approximation . In our studies, we investigated solvable models for the best variational analytical solution for BCS-BEC crossover at T= 0.

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Chapter 1

Introduction and Overview

Particles in nature can be classified as either fermions or bosons depending on their collective behaviors; fermions obey Pauli Exclusion Principle and bosons obey Bose-Einstein statistics and so tend to gather in a same state. One of the most important properties of bosons is the Bose-Einstein Condensation(BEC) where a macroscopic number of particles occupy the lowest energy state at a sufficiently low temperature.This phenomenon was predicted in 1924 and was confirmed experimentally by the observation of superfluidity of ^{4}He in 1938 and later the condensation of ultracold gases in 1995. ^{4}He is a spin zero boson with 2 protons+2 neutrons+2 electrons and ^{3}He is a spin 1/2 fermion with 2 protons+1 neutron+2 electrons. These two isotopes of He are chemically equivalent and have the same atomic spectra but they have completely different properties at low temperatures due to their different statistical nature. They both form superfluid; ^{4}He at 2.17K and ^{3}He at 2mK but the origin and the physical properties of these superfluids are completely different. Fritz London suggested the connection between superfluidity and BEC, but later on superfluid ^{4}He was realized not to be an ideal BEC because of several differences as will be discussed later in this thesis in the BEC chapter.

Superconductivity, namely zero resistivity and perfect diamagnetism in metals is the fermionic equivalent of superfluidity which was first observed in 1911 by Kamerlingh Onnes. Bardeen, Cooper, and Schrieffer (BCS) [9] demonstrated that the superconductivity arises due to the weak electron-electron net attraction propagated by phonons(deformations of the surrounding crystal). In the BCS theory, resistivity goes to zero at low temperatures thanks to the formation of electron pairs which are called *Cooper pairs*[10]. It is commonly said that superconductivity is the result of the BEC of Cooper pairs. However an important difference between BCS superconductivity and BEC is that in the former case attractive interactions are necessary, while even an ideal Bose gas, where there is no interaction whatsoever, can undergo BEC. In 1972 two distinct superfluid phases of ^{3}He were discovered. Since ^{3}He atoms are fermions, these superfluid states were thought to be analog of BCS superconductivity. However, there was no analog of the phonons which provide an attractive potential binding for the Cooper pairs in ^{3}He. The relevant theoretical models have been studied for ^{3}He and it turns out that the Cooper pairs become bound in an l=1 (or p-wave) pairing state instead of usual l=0(s-wave) state.

In the 1980's, Leggett[1], Nozieres and Schmitt-Rink[2] proposed a model unifying BCS and BEC in one single theory. They showed that these two phenomena can be understood as two limiting cases of the ground state of an attractive fermi gas. In the strong interaction regime it corresponds to a BEC of tightly bound dimers, while the weak interaction regime is associated with the BCS state. In between, there are strong many-body quantum correlations which is called BCS-BEC crossover regime.

Recent ultracold atom studies have used *alkali atoms* , since they have a simple electronic structure with a single valence electron. The isotopes of alkali atoms that has even number of neutrons are bosons and the isotopes with odd number of neutrons are fermions since the number of protons is equal to the number of electrons. Therefore ^{87}Rb, ^{85}Rb, ^{23}Na, ^{7}Li, ^{133}Cs are bosons, while ^{6}Li ad ^{40}K are fermions. The experiments showed that the interactions which drive the pairing in ultracold atomic fermions can be controlled by the applied magnetic field. This is the Feshbach resonances which drives the system from BEC type superfluidity to BCS type superfluidity[11, 12] . A Feshbach resonance is a special value of a magnetic field around which small changes in the field strength have dramatic effects on the atomic interactions in an ultracold gas. These resonances occur when the energy associated with the scattering process between two particles becomes close to the energy of a bound state. The dominant interactions in ultracold gases are s-wave collisions whose strength can be described by (E$\approx$ 0) scattering length, a. Across a Feshbach resonance a can be varied from $-\infty$ to $+\infty$ where $a < 0$ and $a > 0$ corresponds to attractive and repulsive interactions respectively. Due to the Zeeman effect by changing the external magnetic field it is possible to control the strength of the interactions, and also whether the interactions are repulsive or attractive. The distinction between BCS and BEC regimes is the energy of the ground states. When the chemical potential, μ, reaches zero, the Fermi surface disappears and a bound state occurs. The minimum of the excitation spectrum changes from finite momentum (BCS limit) to zero momentum (BEC limit), and the excitation gap(energy required to remove a fermion from the superfluid , or create a hole) goes from Δ (BCS limit) to $\sqrt{((\Delta^2) + \mu^2)}$ (BEC limit). In 2003, Deborah Jin and her group at University of Colorado-Boulder achieved the world's first 'fermionic condensate' [13]. In order to form a condensate of a fermi gas of potassium atoms, they changed the external magnetic field to form correlated Fermi atom pairs, which can then act like bosons. Later they could measure the energy of a Fermi gas of atoms for both strong attractive and strong repulsive interactions. And finally they achieved observation of fermionic atom pairs in the BCS-BEC crossover regime[12]

In this thesis, the best variational analytical solution of a BCS-BEC model including crossover problem is presented. Using a simplified model and a trial variational product coherent state of BCS and BEC, we minimized the total energy(diagonal matrix element) for $T = 0$, and by doing that we showed that one can go from BCS limit to BEC limit by variation of the interaction.

In the second chapter of this thesis, Superconductivity is explained starting with phenomenological theory and then the detailed description of BCS Theory is given, and finally liquid ^{3}He is discussed. Chapter 3 starting from historical overview discusses the superfluidity and BEC systems, and ends with a brief discussion on ^{4}He. In chapter 4 the introduction of BCS-BEC crossover phenomenon is given followed by a theoretical approaches, and experimental techniques and results. Chapter 5 starts with the description of coherent state technique in general, and continues with coherent state approach to BCS and BEC systems, and concludes with the application of this technique to crossover problem which we have developed. Finally the last chapter gives the summary of the results we found, open questions and future projects related to this study are discussed.

Chapter 2

BCS

2.1 Historical Overview

Superconductivity, which was first observed by Kamerlingh Onnes in 1911[14], is a phase transition at some critical temperature to a zero resistivity state that most metals, alloys and intermetallic compounds undergo . The superconductive state is one of the first manifestations of a quantum state of macroscopic size, therefore the explanation for this phenomenon had to wait the discovery of the quantum theory (1925) plus 25 years to BCS theory in 1957. What Kamerlingh Onnes observed was that the electrical resistance of various metals disappeared completely at a critical temperature, T_c, which is a characteristic parameter of the material as we know now. He had liquified helium in 1908, and with this new tool to reach low temperatures he started to study the electrical conductivity of metals at lower than 4.2 ^{0}K. He first studied mercury of high purity and observed that the resistance was immeasurably small. An unexpected result he found was that as he added certain non-magnetic impurities to the mercury the resistance didn't increase, moreover the resistance didn't decrease gradually to zero but dropped to zero almost instantly within a narrow temperature range of 0.01 ^{0}K at about 4 ^{0}K, see Fig.(2.1)[15], for the results for Hg.

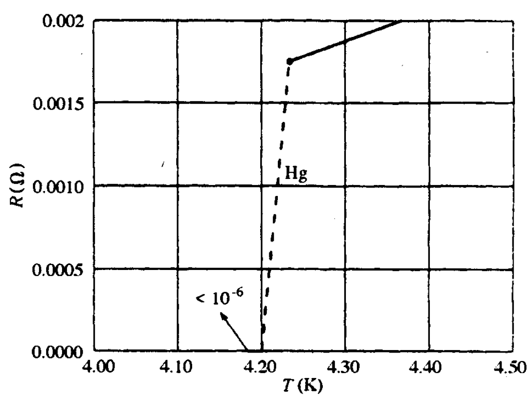

Figure 2.1: The original R vs T graph of mercury by Kamerlingh Onnes,1911

Later on, the complete disappearance of resistivity has been shown with many experiments by observing an electrical current induced in a ring. In a superconducting ring, once a current was induced it has been observed to flow without measurable decrease for a year.

Kamerlingh Onnes also discovered that when the metal is placed in a sufficiently strong magnetic field, superconductivity can be destroyed. However it reappears once the field is removed. The minimum magnetic field required to destroy the superconductivity depends on the shape and the material at hand. This transition is sharp and the critical field,H_c, depends on the temperature. It is zero at the critical temperature and increases with the increasing temperature. The temperature dependence of H_c for most superconductors can be given as:

$$\frac{H_c(T)}{H_c(0)} = 1 - \left(\frac{T}{T_c}\right)^2 \tag{2.1}$$

While the transition at zero field at T_c is second order, the transition in the presence of a field is first order since there is a discontinuous change in the thermodynamic state of the system, and an associated latent heat.

If we describe a superconductor by an infinite conductivity, the electric field inside must always be zero, which leads to the fact that the magnetic induction is constant in time

$$\frac{\partial \mathbf{B}}{\partial t} = 0 \tag{2.2}$$

due to the Maxwell equation:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{2.3}$$

Meaning that the magnetic induction inside depends on the past history of the state.This can be tested by preparing a sample in two different ways:

first the sample can be prepared in an external magnetic field H_0 and then the temperature is decreased below T_c, or the sample can be cooled down below T_c first and then the magnetic field turned on. In the first case, the induction inside should remain at H_0, while in the second case it should remain zero. But if that's true, then it means that the superconducting state is not unique for a given external magnetic field, therefore the equilibrium thermodynamics laws can't be applied. However, according to an observation which was made in 1933 by Meissner and Ochsenfeld, the magnetic induction inside a superconductor is *always* zero, B= 0, in all circumstances. In their experiments, Meissner and Ochsenfeld showed that as the sample is cooling off below T_c the magnetic field is expelled in the first type of experiments. In order to maintain $\mathbf{B} = 0$ inside at all times, there should be some screening currents flowing on the surface of the superconductor which produces a magnetic field of equal magnitude and opposite direction to the external magnetic field. This can be explained by using Maxwell's equation, and separating the total current into externally applied and internal screening currents;

$$\mathbf{j} = \mathbf{j_{ext}} + \mathbf{j_{int}} \tag{2.4}$$

and we know that the screening currents create a magnetization on the surface of the sample;

$$\nabla \times \mathbf{M} = \mathbf{j}_{int} \tag{2.5}$$

and we define the magnetic field as;

$$\nabla \times \mathbf{H} = \mathbf{j}_{ext} \tag{2.6}$$

The relation between **B**,**H** and **M** is:

$$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M}) \tag{2.7}$$

and with the Maxwell's equation;

$$\nabla \cdot \mathbf{B} = 0 \tag{2.8}$$

we can find the boundary conditions;

$$\Delta \mathbf{B}_{\perp} = 0 \tag{2.9}$$

$$\Delta \mathbf{H}_{\parallel} = 0 \tag{2.10}$$

Imposing the Meissner condition $\mathbf{B} = 0$ we obtain;

$$\mathbf{M} = -\mathbf{H} \tag{2.11}$$

and the definition of diamagnetic susceptibility;

$$\chi = \frac{dM}{dH} \tag{2.12}$$

leads us to the conclusion that the diamagnetic susceptibility is -1 in Gaussian, or $-1/4\pi$ in cgs, units for superconductors. This shows us why superconductors are perfect diamagnets and therefore the external magnetic fields are completely screened out.

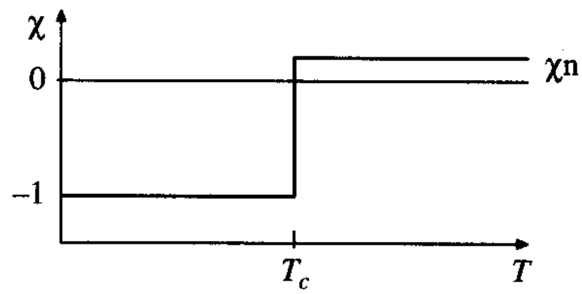

Figure 2.2: χ vs T [4]

With this result, we can now securely say that the superconducting state is a single thermodynamically stable state and the laws of thermodynamics apply as they do to any phase. Moreover, it is believed that susceptibility measurement is more reliable evidence for superconductivity than zero resistance and therefore superconductors are described as perfect diamagnets as well as a perfect conductor. However, perfect diamagnetism and infinite conductivity are independent properties of superconductors, neither implying the other.

The first theory about the magnetic properties of superconductors was developed by two brothers F.London and H.London in 1935. They assumed that some fraction of the conduction electrons become superfluid while the rest remain normal, and the superfluid electrons move without resistivity and naturally short circuit the normal ones, making the overall resistivity zero at all times. Let's start with the equation of motion for electrons in a metal;

$$m\left(\frac{d\mathbf{v}}{dt}+\frac{\mathbf{v}}{\tau}\right)=e\mathbf{E} \tag{2.13}$$

For a perfect conductor τ (the scattering time) would be ∞ and with the definition of current density, $\mathbf{j} = ne\mathbf{v}$, where n is the number density of superconducting electrons, we can rewrite this equation as:

$$\frac{d\mathbf{j}}{dt}=\left(\frac{ne^2}{m}\right)\mathbf{E} \tag{2.14}$$

which is known as the first London equation.

The fourth Maxwell's equation gives us:

$$\nabla\times\frac{\partial B}{\partial t}=\mu_o\frac{\partial j}{\partial t}+\frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} \tag{2.15}$$

Using the first London equation we can rewrite this as:

$$\nabla\times\left(\nabla\times\frac{\partial B}{\partial t}\right)=\left(\frac{\mu_o ne^2}{m}+\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\nabla\times\mathbf{E} \tag{2.16}$$

and using the third Maxwell's equation(eq.(2.3)):

$$\nabla\times\left(\nabla\times\frac{\partial B}{\partial t}\right)+\left(\frac{\mu_o ne^2}{m}+\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\frac{\partial B}{\partial t}=0 \tag{2.17}$$

Here we can introduce the London depth (or penetration depth),λ_L, by:

$$\lambda_L = \left(\frac{m}{\mu_o n e^2}\right)^{1/2} \tag{2.18}$$

which is the distance inside the surface over which an external magnetic field is screened out to zero. As a result, the second London equation can be written as:

$$\nabla \times (\nabla \times \mathbf{B}) + \left(\frac{1}{\lambda_L^2} + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{B} = 0 \tag{2.19}$$

Meissner effect can be explained by thinking of a superconductor in a magnetic field near a plane boundary. For a field perpendicular to the superconducting surface, let's say lying in the x-y plane with no current flowing in the z direction, the second Maxwell's equation suggest that $\nabla \cdot \mathbf{H}$=0 giving us $\frac{\partial H_z}{\partial z} = 0$ or H=const. From the fourth Maxwell's equation we know that $\nabla \times \mathbf{B}$=0 which then yields $\mathbf{B}$=0 telling us that a superconductor cannot have a field component perpendicular to its surface. However for a field lying parallel to the surface, $\mathbf{B} = B(z)\hat{\mathbf{x}}$, we can write the second London equation using the vector identity:

$$\nabla \times (\nabla \times \mathbf{B}) = \nabla(\nabla \cdot \mathbf{B}) - \nabla^2\mathbf{B} \tag{2.20}$$

$$\frac{\partial^2 H_x}{\partial z^2} - \frac{1}{\lambda_L^2}H_x = 0 \tag{2.21}$$

which has a nonzero solution that decays exponentially with λ_L, which means a field parallel to the surface is allowed in this London-Maxwell model. This parallel field is a surface current density which screens the magnetic field from the interior of the superconductor. Depending on the material, at T=0, the penetration depth ranges from 500 to 10,000$\AA$.

For static fields the London equation can be written as:

$$\nabla \times (\nabla \times \mathbf{B}) = -\frac{1}{\lambda_L^2}\mathbf{B} \tag{2.22}$$

By using the magnetic vector potential, $\mathbf{A}$, which is restricted to the gauge $\nabla \cdot \mathbf{A} = \mathbf{0}$ (London gauge), where $\mathbf{B} = \nabla \times \mathbf{A}$, we can write:

$$\mathbf{j} = -\frac{1}{\mu_o \lambda_L^2}\mathbf{A} \tag{2.23}$$

Later on a modified form of London equation was proposed by Pippard. He suggested that the current $\mathbf{j}(\mathbf{r})$ at a point r involves contributions from $\mathbf{A}(\mathbf{r}')$ at neighboring points r$'$ located in a volume with a radius of order ξ_o surrounding r. Here ξ_o is the coherence length give by:

$$\xi_o = \frac{\hbar v_F}{\pi \Delta} \tag{2.24}$$

where v_F is the fermi velocity, and Δ is the energy gap which will be explained later in the BCS Theory. Here let's make a short remark that this coherence length also represents the physical size of the Cooper pair. The expression Pippard suggested was:

$$\mathbf{j}(\mathbf{r}) = -\frac{ne^2}{m}\frac{3}{4\pi\xi_o}\int \frac{\mathbf{R}(\mathbf{R}\cdot\mathbf{A}(\mathbf{r}'))}{R^4}e^{-R/r_o}d^3r' \tag{2.25}$$

where $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ and r_o is defined to account for the scattering of electrons when the metal has impurities and it is given by:

$$\frac{1}{r_o} = \frac{1}{\xi_o} + \frac{1}{l} \tag{2.26}$$

here $l = v_F\tau$ is the electron mean free path at the fermi surface. In the limit $\lambda_L \gg \xi_o$ eq.(2.25) reduces to the London equation. In the other limit, $\lambda_L \ll \xi_o$, we may need corrections to the London equation since $\mathbf{A}(\mathbf{r}')$ varies rapidly.

We have seen three different length scales which characterizes a superconductor; the London penetration depth(λ_L), the Cooper pair coherence length(ξ_o), and the Drude mean free path(l). Comparison of these length scales can tell us what type of superconductor we have. For example, if $\lambda_L < \xi_o$ the superconductor is called type-I (Pippard type), and if $\lambda_L > \xi_o$, then it is called type-II (London type) superconductor. Similarly, if we have $l > \xi_o$, the superconductor is said to be in the clean limit, while if we have $l < \xi_o$, it is said to be in the dirty limit. The detailed description of these types and limits of the superconductors is given in the following pages.

The diamagnetic susceptibility argument which we have discussed previously is true for small external fields, but it has been shown that as the applied field is increased there are two possible scenarios. For some superconductors as the applied field is increased the **B** field remains zero until the superconductivity is destroyed suddenly: these type superconductors are called type-I. For type-II superconductors there are two critical magnetic fields; as the applied field is increased, at the lower critical field, H_{c1}, the magnetic flux starts to enter the superconductor and as the external field increases more the magnetic flux density increases gradually until at the upper critical field, H_{c2}, the superconductivity is destroyed as shown in the Figure 2.3

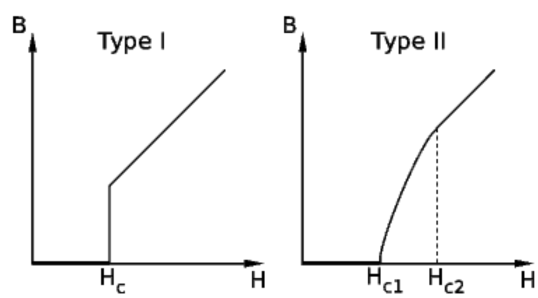

Figure 2.3: B vs H for $T < T_c$

The explanation of the state between H_{c1} and H_{c2}, which is a mixture of normal and superconducting phase, was given by Abrikosov in 1957(the same year as BCS). He showed that the magnetic field can enter into the superconductor in the form of vortices where each vortex has a cylindrical normal electronic core around which a supercurrent is circulating and the field enters through this normal core by a fixed unit of flux, $\phi_o = h/2e$ per vortex line. The number of vortices increases with increasing magnetic field. The radius of each vortex is approximately the coherence length (ξ_o), and outside the vortex core we can still use the London equation.

In 1950, Ginzburg and Landau gave the thermodynamic description of superconducting phase transition, which is known as GL theory [16]. Although this theory describes low-T_c superconductors almost perfectly, it fails for the new high-T_c superconductors as it is a mean field theory and neglects the thermal fluctuations which is very important for the latter case. In this theory in order to describe the phase transition they introduced a complex pseudowave function ψ as an order parameter which describes the superconducting electrons as well as the local density of superconducting electrons as:

$$n_s = |\psi(x)|^2 \tag{2.27}$$

Later on it was shown that ψ is directly proportional to the gap parameter,Δ, and it is the wavefunction of the center of mass motion of Cooper pairs[15].

Using a variational principle, they derived the following equation for ψ:

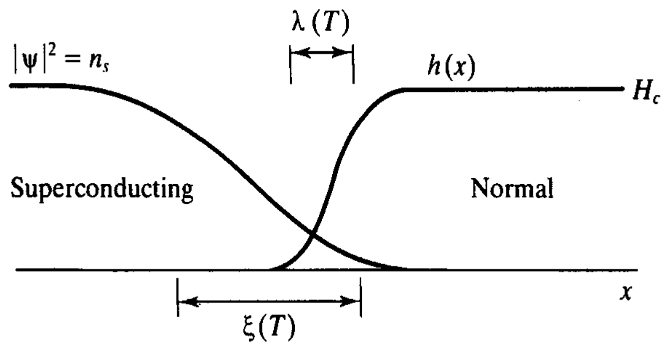

Figure 2.4: Intermediate state between superconducting and normal phases

$$\frac{1}{2m^*}\left(\frac{\hbar}{i}\nabla - \frac{e^*}{c}A\right)^2\psi + \beta|\psi|^2\psi = -\alpha(T)\psi \tag{2.28}$$

which is the Schrödinger equation for a free particle with a nonlinear term. Then they introduced a characteristic length, which is know as the GL coherence length;

$$\xi(T) = \frac{\hbar}{|2m^*\alpha(T)|^{1/2}} \tag{2.29}$$

In the limit $T \ll T_c$, $\xi(T) \approx \xi_o$ and therefore temperature independent, while around T_c, $\xi(T)$ diverges since $\alpha(T)$ vanishes as T approaches to T_c. Therefore they redefined their characteristic length to introduce a dimensionless parameter;

$$\kappa = \frac{\lambda}{\xi} \tag{2.30}$$

Here λ is the penetration depth which we know at T=0 as eq.(2.18), and since the temperature dependence of both λ and ξ diverges as $(T - T_c)^{-1/2}$ near T_c, the GL parameter,κ, is approximately independent of temperature. In his work, Abrikosov[17] showed that for materials with $\kappa > 1/\sqrt{2}$ instead of a discontinuous breakdown of superconductivity there was a continuous increase in flux penetration starting at H_{c1} and reaching $B = H$ at H_{c2}, hence the value $\kappa = 1/\sqrt{2}$ separates superconductors of type-I and type-II.

2.2 BCS Theory

The first microscopic explanation for superconductivity was given by Bardeen-Cooper-Schrieffer (BCS) in 1957[9]. The basic idea behind the BCS theory was proposed by Cooper in 1956[10], he showed that for a system of electrons (i.e. fermions) no matter how weak is the electron-electron attraction, the Fermi sea of electrons is unstable against the formation of bound pairs now called Cooper pairs. In his work he put two extra electrons to a Fermi sea at $T = 0$ and assumed that these electrons interact only with each other but not with others except via the Pauli exclusion principle. So he wrote the two-particle wavefunction with the condition that the total momentum and spin is equal to zero, meaning that the two electrons have equal and opposite momenta, hence the center of mass of the pair is at rest with respect to the Fermi sea.

$$\psi_o(r_1, r_2) = \sum_k g_k e^{ik\cdot r_1} e^{-ik\cdot r_2} \tag{2.31}$$

and because of the fermi nature of electrons the antisymmetry of total wavefunction with respect to exchange of electrons ψ_0 should be written as either a sum of products of $\cos k \cdot (r_1 - r_2)$ with antisymmetric singlet spin function or as a sum of products of $\sin k \cdot (r_1 - r_2)$ with symmetric triplet spin function. Since the attractive interaction is required, singlet coupling would have a lower energy, which makes our Cooper pair wavefunction;

$$\psi_o(r_1 - r_2) = \left[\sum_{k>k_F} g_k cos k \cdot (r_1 - r_2)\right] [\sigma_{1\uparrow}\sigma_{2\downarrow} - \sigma_{1\downarrow}\sigma_{2\uparrow}] \tag{2.32}$$

The Schrödinger equation for the pair wavefunction is:

$$\left[-\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + V(r_1, r_2)\right] \psi_o(r_1, r_2) = \left[\varepsilon + 2\frac{\hbar^2 k_F^2}{2m}\right] \psi_o(r_1, r_2) \tag{2.33}$$

Substituting the pair wavefunction into this:

$$\frac{\hbar^2 k^2}{m} g(k) + \sum_{k'} g(k') V_{k,k'} = (\varepsilon + 2\varepsilon_F) g(k) \tag{2.34}$$

where $V_{k,k'}$ characterizes the strength of the potential for scattering of two electrons and given by:

$$V_{k,k'} = \frac{1}{L^3} \int V(r) e^{i(k'-k)\cdot r} d^3 r \tag{2.35}$$

where r is the distance between the two electrons and L_3 is the normalization volume. Because of the exclusion principle and the assumption of a filled Fermi sea $g(k) = 0$ for $k < k_F$. For simplification Cooper introduced the cutoff energy in such a way that:

$$V_{k,k'} = \left\{ \begin{array}{c} -\frac{V}{L^3}, \mid \frac{\hbar^2 k^2}{2m} - \varepsilon_F \mid and \mid \frac{\hbar^2 k'^2}{2m} - \varepsilon_F \mid < \hbar\omega_c, \\ 0, \mid \frac{\hbar^2 k^2}{2m} - \varepsilon_F \mid or \mid \frac{\hbar^2 k'^2}{2m} - \varepsilon_F \mid > \hbar\omega_c \end{array} \right\} \tag{2.36}$$

Then calculating the integral one can obtain:

$$\left(-\frac{\hbar^2 k^2}{m} + \varepsilon + 2\varepsilon_F \right) g(k) = -\frac{V}{L^3} \sum_{k'} g(k') \tag{2.37}$$

Summing both sides over k one can show that we obtain:

$$1 = \frac{V}{L^3} \sum_{k} \frac{1}{\left(\frac{\hbar^2 k^2}{m} - \varepsilon - 2\varepsilon_F \right)} \tag{2.38}$$

and writing $\xi = \hbar^2 k^2 2m - \varepsilon_F$ and converting the sum to integral, and using the density of states per spin:

$$V \int_0^{\hbar\omega_c} \frac{n(\xi)d\xi}{2\xi - \varepsilon} = 1 \tag{2.39}$$

Here, $n(\xi)$ can be taken as $n(0)$ (density of states per spin at the Fermi surface) over the integration range and carrying out the integration gives:

$$\frac{1}{2} n(0) V ln \left(\frac{\varepsilon - 2\hbar\omega_c}{\varepsilon} \right) = 1 \tag{2.40}$$

assuming $|\varepsilon| \ll \hbar\omega_c$ this equation can be solved as:

$$\varepsilon = -2\hbar\omega_c e^{\frac{2}{n(0)V}} \tag{2.41}$$

With this result Cooper showed that there is a bound state with a negative energy (note that $\varepsilon < 0$) with respect to the Fermi surface. The bound states are filled with electrons whose energy is greater than the Fermi energy,$k > k_F$, and because the attractive potential energy is greater than this extra kinetic energy the total energy of a pair becomes negative leading to a bound state. This bound state suggests a gap (Δ) in the energy spectrum which was observed in experiments. Moreover, this bound state was obtained regardless of how small V is, and there is a bound state only if the attraction is greater than a minimum energy. Finally, note that this expression for binding energy cannot be written in powers of V because it has an essential singularity at $n(0)V = 0$ and that's why it couldn't be obtained by any perturbation method.

The reason behind this attractive potential between two electrons is not so obvious at first sight, since two *free* electrons repel each other due to the Coulomb interaction. However, when two electrons are in a lattice, being *valance* electrons they interact with their environment in such a way that the first electron attracts the positive ions around it, then this positive ion cloud attracts the second electron giving an effective attractive interaction between these two electrons. When this attractive interaction becomes stronger than the Coulomb one superconductivity results. Historically, the explanation of superconductivity by the electron-lattice interaction was first given by Fröhlich in 1950. When an electron is scattered from a state of momentum $\mathbf{k}$ to a state of momentum $\mathbf{k}'$, while interacting with ions, the relevant phonon will have the momentum $\mathbf{q} = \mathbf{k} - \mathbf{k}'$, and the phonon frequency is ω_q, then the phonon contribution to the screening will be proportional to $(\omega^2 - \omega_q^2)^{-1}$, and obviously for $\omega < \omega_q$ this term will be negative. Therefore, for electron energy differences larger than $\hbar\omega_q$ the interaction will be repulsive, and the cutoff energy, $\hbar\omega_c$ of Cooper's attractive potential is clearly in the order of the Debye energy, $\hbar\omega_c = k\Theta_D$.

At this point, it is important to note that the basis of superconductivity is the attractive potential energy between two electrons which is due to the phonon exchange for classic superconductors. But for exotic superconductors, like organic, heavy fermion, high T_c superconductors, newly found iron-arsenic pnictides, the origins of the pairing interaction is still under argument, and two probable origin mentioned in debates are boson (magnon, plasmon, exciton) exchange, and spin exchange. Another difference between classical superconductors and new exotic ones is that the latter don't show the "ideal" BCS isotope effect which is one of the most important properties that the BCS theory explains correctly. To be more correct, a recent work showed that the Fe-pnictides exhibits the isotope effect [18]. This effect was observed by many experimentalist as early as 1950, and it simply relates the critical temperature with the isotopic mass of the constituents with the relation:

$$T_c = M^{-\alpha} \tag{2.42}$$

α was predicted to be 1/2 by BCS theory which agrees with the most common s-wave conventional superconductors. The absence of the usual BCS isotope effect might be an indication that the lattice phonons are not involved in the pairing mechanism for exotic superconductors, or involved in some new fashion.

Now, going back to the BCS wave function, we know that that the Fermi sea is unstable against the formation of Cooper pairs, so we will write the many body ground state wave function by using pairs of electrons as:

$$\psi_N = \sum_{k_1} ... \sum_{k_{N/2}} g_{k_1}...g_{k_{N/2}} \hat{A}(e^{ik_1\cdot(r_1-r_2)}...e^{ik_{N/2}\cdot(r_{N-1}-r_N)}) \times [\sigma_{1\uparrow}\sigma_{2\downarrow}...\sigma_{N-1\uparrow}\sigma_{N\downarrow}] \tag{2.43}$$

where $\hat{A}$ is the antisymmetrization operator, and only the spin singlet pairing is used. Obviously, usage of second quantization technique is going to make life easier, therefore for that purpose we will introduce the fermi creation and annihilation operators which satisfy the anticommutation relations:

$$[\hat{a}^{\dagger}_{k\sigma 1}, \hat{a}_{k'\sigma 2}]_{+} = \delta(k, k^{'})\delta(\sigma 1, \sigma 2) \tag{2.44}$$

$$[\hat{a}_{k}, \hat{a}_{k'}]_{+} = 0 \tag{2.45}$$

$$[\hat{a}^{\dagger}_{k}, \hat{a}^{\dagger}_{k'}]_{+} = 0 \tag{2.46}$$

In the second quantization notation the many body wave function is written as:

$$|\psi_N\rangle = \sum_{k_1} ... \sum_{k_{N/2}} g_{k_1}...g_{k_{N/2}} (\hat{a}^{\dagger}_{k_1\uparrow}\hat{a}^{\dagger}_{-k_1\downarrow}...\hat{a}^{\dagger}_{k_{N/2}\uparrow}\hat{a}^{\dagger}_{-k_{N/2}\downarrow}) |\phi_0\rangle \tag{2.47}$$

where $|\phi_0\rangle$ is the vacuum state. However, even this wavefunction is too hard to work with, therefore BCS proposed an alternative wavefunction:

$$|\psi_{BCS}\rangle = \prod_k (u_k + v_k \hat{a}^\dagger_{k\uparrow} \hat{a}^\dagger_{-k\downarrow}) |\phi_0\rangle \tag{2.48}$$

The difference between these two states eq.2.47 and eq.2.48 is that the first one describes exactly pair of N/2 electrons while the second one doesn't have any constraint on the number of electrons, but since the number of electrons is huge this difference doesn't cause a serious error in calculations of some properties of superconductors. We can relate these two wavefunctions by:

$$|\psi_{BCS}\rangle = \sum_N \lambda_N |\psi_N\rangle \tag{2.49}$$

where the values of $|\lambda_N|^2$ are peaked at $\bar{N}$, and $\sum_N |\lambda_N|^2 = 1$ due to the normalization condition.

The average number of particles, $\bar{N}$,associated with the BCS wavefunction can be calculated as:

$$\bar{N} = \langle\psi_{BCS}| \hat{N} |\psi_{BCS}\rangle = \sum_k 2|v_k|^2 \tag{2.50}$$

where $\hat{N}$ is defined as the number operator:

$$\hat{N} = \sum_{k,\sigma} \hat{a}^\dagger_{k\sigma} \hat{a}_{k\sigma} \tag{2.51}$$

In the Cooper description at $T = 0$ all states with $|k| < k_F$ are filled and those with $|k| > k_F$ are empty, which means that:

$$u_k = 0, v_k = 1, |k| < k_F,$$

$$u_k = 1, v_k = 0, |k| > k_F$$

and the normalization condition for BCS wavefunction yields:

$$\langle \psi_{BCS} | \psi_{BCS} \rangle = 1 \tag{2.52}$$

which reads:

$$|u_k|^2 + |v_k|^2 = 1 \tag{2.53}$$

The pairing Hamiltonian of the system of electrons can be written as:

$$\hat{H}_{BCS} = \sum_{k,\sigma} \epsilon_k \hat{a}^\dagger_{k,\sigma} \hat{a}_{k,\sigma} + \sum_{k,k'} V_{k,k'} \hat{a}^\dagger_{k\uparrow} \hat{a}^\dagger_{-k\downarrow} \hat{a}_{-k'\downarrow} \hat{a}_{k'\uparrow} \tag{2.54}$$

where $\epsilon_k = \hbar^2 k^2 / 2m$, and only the opposite momenta and opposite spin particles were considered which makes this Hamiltonian *reduced*.

The constraint that the average number of electrons is $\bar{N}$ should be imposed through a Lagrange multiplier μ (i.e. the chemical potential which is equal to ϵ_F at $T = 0$). This defines the reduced Hamiltonian:

$$\hat{H}'_{BCS} = \hat{H}_{BCS} - \mu \hat{N} = \sum_{k,\sigma} \xi_k \hat{a}^\dagger_{k,\sigma} \hat{a}_{k,\sigma} + \sum_{k,k'} V_{k,k'} \hat{a}^\dagger_{k\uparrow} \hat{a}^\dagger_{-k\downarrow} \hat{a}_{-k'\downarrow} \hat{a}_{k'\uparrow} \tag{2.55}$$

where $\xi_k = \hbar^2 k^2/2m - \mu$. However this term needs a correction due to the many body correlations; in this system electrons are no longer free and $\hat{a}^\dagger$ operators create quasiparticles with an effective mass of m^*, therefore $\xi_k = \hbar^2 k^2/2m^* - \mu = \hbar^2(k^2 - k_F^2)/2m^*$ with k_F being the Fermi wave vector. Note that one can define "pair operators" (as did BCS) by $b^\dagger = a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}$, $b = a_{-k\downarrow} a_{k\uparrow} = (b^\dagger)^\dagger$ and do the analysis using them.

The expectation value of the reduced Hamiltonian is:

$$\langle\psi_{BCS}|\, \hat{H'}_{BCS}\, |\psi_{BCS}\rangle = 2\sum_k \xi_k v_k^2 + \sum_{k,k'} V_{k,k'} u_k v_k u_{k'} v_{k'} \tag{2.56}$$

For simplicity, u_k and v_k is chosen to be real and in the form:

$$u_k = cos\theta_k$$

$$v_k = sin\theta_k$$

to ensure the normalization condition. With this definition, we can rewrite the energy eigenvalue as:

$$\langle\psi_{BCS}|\, \hat{H'}_{BCS}\, |\psi_{BCS}\rangle = 2\sum_k \xi_k sin^2\theta_k + \frac{1}{4}\sum_{k,k'} V_{k,k'} sin2\theta_k sin2\theta_{k'} \tag{2.57}$$

Minimization with respect to θ_k yields:

$$\frac{\partial}{\partial\theta_k}\langle\psi_{BCS}|\, \hat{H'}_{BCS}\, |\psi_{BCS}\rangle = 2\xi_k sin2\theta_k + \sum_{k'} V_{k,k'} cos2\theta_k sin2\theta_{k'} = 0 \tag{2.58}$$

from which we can write:

$$\xi_k tan2\theta_k = -\frac{1}{2}\sum_{k'} V_{k,k'} sin2\theta_{k'} \tag{2.59}$$

Here if the *gap* function is defined as:

$$\Delta_k = -\frac{1}{2}\sum_{k'} V_{k,k'} sin2\theta_{k'} = -\sum_{k'} V_{k,k'} u_{k'} v_{k'} \tag{2.60}$$

then eq.2.59 can be written as:

$$tan2\theta_k = \frac{\Delta_k}{\xi_k} \tag{2.61}$$

Furthermore, this equation enables us to write:

$$\epsilon_k = (\xi_k^2 + \Delta_k^2)^{1/2} \tag{2.62}$$

with the fact that:

$$sin2\theta_k = \frac{\Delta_k}{\epsilon_k} \tag{2.63}$$

and

$$cos2\theta_k = \frac{\xi_k}{\epsilon_k} \tag{2.64}$$

From these last two equations one can easily deduce that:

$$u_k^2 = \frac{1}{2}\left(1 + \frac{\xi_k}{\epsilon_k}\right) \tag{2.65}$$

and

$$v_k^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{\epsilon_k}\right) \tag{2.66}$$

Finally, returning back to the definition of the *gap* one can write the gap equation:

$$\Delta_k = -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2\epsilon_{k'}} = -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2(\xi_{k'}^2 + \Delta_{k'}^2)^{1/2}} \tag{2.67}$$

This is a nonlinear integral equation which has a trivial solution at $T = 0$, $\Delta_k = 0$ (where all the states are filled up to the normal Fermi sea), and it has also a nontrivial solution for $V_{k,k'} < 0$ with a lower energy which was obtained by BCS with the model potential which was proposed by Cooper earlier (eq.2.36):

$$V_{k,k'} = \left\{ \begin{array}{c} -V, \mid \xi_k \mid and \mid \xi_{k'} \mid \leq \hbar\omega_D, \\ 0, \mid \xi_k \mid or \mid \xi_{k'} \mid \geq \hbar\omega_D \end{array} \right\} \tag{2.68}$$

Using this potential one can write the gap function as:

$$\Delta_k = \left\{ \begin{array}{c} \Delta, \xi_k < \hbar\omega_D, \\ 0, \xi_k > \hbar\omega_D \end{array} \right\} \tag{2.69}$$

Since Δ_k is independent of k, one can take Δ out of the summation and cancel it from both sides in eq.2.67 and replacing the summation with integral:

$$1 = N(0)V \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\varepsilon}{2(\xi^2 + \Delta^2)^{1/2}} \tag{2.70}$$

which then gives:

$$1 = N(0)V \sinh\left(\frac{\hbar\omega_D}{\Delta}\right) \tag{2.71}$$

where N(0) is the density of states at the Fermi energy.

As a result, using the weak coupling limit $N(0)V \ll 1$, the gap function at $T = 0$ is found to be:

$$\Delta = \frac{\hbar\omega_D}{\sinh(\frac{1}{N(0)V})} \approx 2\hbar\omega_D e^{-1/N(0)V} \tag{2.72}$$

It is clear that there is always a solution for the gap equation no matter how small is the attractive potential,V.

Now it can be shown that the ground state energy for BCS state is lower than the Fermi sea state.

$$\langle\psi_{BCS}|\, \hat{H}_{BCS} - \mu\hat{N}\, |\psi_{BCS}\rangle = \sum_k \left(\xi_k - \frac{\xi_k^2}{\epsilon_k}\right) - \frac{\Delta^2}{V} \tag{2.73}$$

The normal state at $T = 0$ for a superconductor, is the BCS state with $\Delta = 0$, which then reads:

$$E_n = \langle\psi_{BCS}|\, \hat{H}'_{BCS}\, |\psi_{BCS}\rangle_n = \sum_{|k|<k_F} 2\varepsilon_k \tag{2.74}$$

where $\epsilon_k = |\xi_k|$ which means that the excitation energies are $+\xi_k$ for adding an electron, and -ξ_k for removing an electron(or adding a hole) to an empty normal state.

The energy difference between the normal ground state and the superconducting ground state can be calculated as:

$$E_s - E_n = \sum_k \xi_k \left(1 - \frac{\xi_k}{\epsilon_k}\right) - \frac{1}{4} V \sum_{k,k'} \frac{\Delta^2}{\epsilon_k \epsilon_{k'}} - \sum_k \xi_k \left(1 - \frac{\xi_k}{|\xi_k|}\right) \tag{2.75}$$

where eq.(2.56) is used for E_s. Changing the summations to integrals and using eq.(2.70) this can be written as:

$$E_s - E_n = N(0) \int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi \left(|\xi| - \frac{\xi^2}{\epsilon}\right) - \frac{N(0)}{2} \Delta^2 \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\xi}{\epsilon} \tag{2.76}$$

$$\approx 2N(0) \int_0^\infty d\xi \left(\xi - \frac{\xi^2}{\epsilon} - \frac{\Delta^2}{2\epsilon}\right) \tag{2.77}$$

$$= -\frac{1}{2} N(0) \Delta^2 \tag{2.78}$$

which is always negative confirming that the superconducting state has a lower energy than the normal state.

2.3 ^{3}He : An "Analog" system to Metallic BCS

The first observation of two (of the three) novel phase transitions in ^{3}He was made by Lee,Oscheroff, and Richardson at Cornell in 1972. It was shown that these phases are two different superfluids, which are called A and B phases, and the transition temperature is around 2-3mK, see Fig.2.5

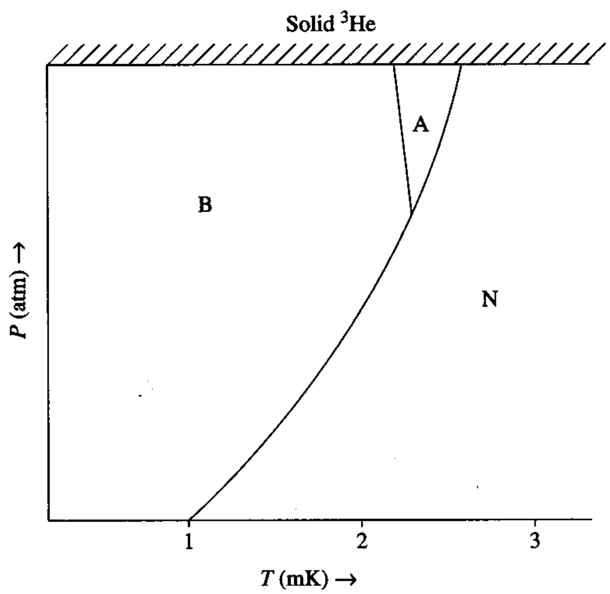

Figure 2.5: Three phases of ^{3}He: A and B(superfluid), N(normal).[1]

Since ^{3}He atoms are fermions, it was suggested that these phases are analogs of BCS superconductivity, but soon it was discovered that in ^{3}He there is no analog of the phonons which binds the Cooper pairs in BCS systems. Later on it was observed that unlike the Cooper pairs in classic superconductors, which are formed in s-wave state with a definite structure at a given temperature and pressure, the anomalous phases of liquid ^{3}He are formed in p-wave pairing state having a nontrivial internal structure which can change in time and space.

Liquid ^{3}He shows characteristic degenerate Fermi gas behavior below ∼100mK, while the values of c_V, χ,etc. shows different behavior than a degenerate non-interacting gas, and these behaviors are explained by the Fermi-liquid theory by Landau.

If we assume that the particle interactions $V(r_i - r_j)$ is negligibly small at $T = 0$, the ground state can be written simply by occupying all the states up to a Fermi surface. Since the liquid ^{3}He is isotropic the Fermi surface must be a sphere with radius k_F, where $k_F = (3\pi^2 n)^{1/3}$. Mass density of ^{3}He is 81kg/m^3 which gives us k_F=0.78$\mathring{A}^{-1}$ and a Fermi energy of 0.49meV(≡4.9K). This is thousand times greater than the energy of superfluid ^{3}He which tells us that the system is degenerate Fermi gas. On the other hand, the particle interactions in ^{3}He is far from being negligible that we can say it is a very dense fluid of *perfectly* hard spheres. The basic idea behind the Fermi liquid theory is that even though the particles are strongly interacting, the excitations relative to the ground state act as weakly interacting particles which are called *quasiparticles*. A quasiparticle with spin $\sigma =\uparrow$ causes a local polarization of the neighboring quasiparticles due to the Pauli exchange interaction which is the dominant spin-spin interaction in ^{3}He. The Pauli exclusion principle forces the parallel spins to be separated in space leading to *exchange* energy which causes spins to be aligned ferromagnetically, and this attractive interaction leads to a Cooper instability.

In superfluid ^{3}He the pairing of quasiparticles is in spin triplet state(p-wave pairing) in contrary to the classic BCS superconductors which has spin singlet pairing(s-wave pairing) of Cooper pairs. This difference originates from the different interaction potentials; while the BCS pairing potential is strongly attractive for all k vectors near Fermi surface, the quasiparticle interactions at the Fermi level are both k and spin dependent.

Chapter 3

BEC

3.1 Historical Overview

Based on a paper by S.N.Bose (1924)[19], in 1925 A.Einstein[20] published a paper in which he proposed that below a certain temperature, a gas of non-interacting bosonic atoms would undergo a phase transition and populate the lowest energy state macroscopically, which is called Bose-Einstein condensation (**BEC**). At the end of 1938, when P. Kapitza[21] , and separately J.F. Allen and A.D.Misener[22] observed that ^{4}He flows without dissipation (i.e. without losing energy) below a certain temperature, F.London[23] immediately proposed that this was the manifestation of BEC since ^{4}He atom is a boson. However, later on, it was shown that there are several major differences between ^{4}He gas and a noninteracting boson gas which leads researchers to focus on the superfluidity of ^{4}He and a comprehensive theory including interactions on ^{4}He was proposed by Landau[24] in 1941. In 1947 Bogoliubov[25] developed a microscopic theory of interacting Bose gases, and in 1951 the concept of off-diagonal long range order (ODLRO) was introduced by Landau-Lifshitz[26], and Penrose[27] and Penrose-Onsager[28]. ODLRO can be understood as nonzero off-diagonal density matrix element at large distances in the presence of BEC, meaning that the process including absorption of a particle at point r into the condensate and simultaneously creation of a second particle at another point r' out of condensate has a non-zero quantum mechanical amplitude. This is because of the quantum coherence of the condensate, and this amplitude is independent of the distance between points r and r'. With this concept at hand a huge amount of theoretical work was developed. An important development about the relation between BEC and superfluidity was achieved with the prediction of quantized vortices by Onsager (1949)[29] and Feynman(1955)[30] and the experimental observation was achieved in 1956 by Hall and Vinen[31].

Although many experiments were performed after the theoretical proposal of BEC, the experimental confirmation was achieved for the first time in 1995 in ultra-cold rubidium and sodium atom vapors [32–34], and for this achievement Cornell, Wieman, and Wolfgang Ketterle was awarded the 2001 Nobel Prize in Physics. The late confirmation is due to the fact that the

BEC theory was proposed for the ideal (noninteracting) bosonic gas which is realized to be a good approximation in a gas of very dilute alkali metal atoms, while the atomic masses for alkali metals are high which causes very low critical temperature values of the order of 10nK-10μK, and achieving these low temperatures needed very sophisticated experimental techniques. The alkali atoms has interatomic interactions which can be very strong at short distances. Moreover, at large interatomic distances van der Waals attraction causes the atoms to bind together strongly but this process takes a long time due to the fact that the most of the collisions are two body elastic collisions which can't result in binding the atoms. Specifically, at the low density limit three-body collision rate is very small. Therefore, the atoms can be kept in the trapped state long enough to make the necessary measurements. Since alkali atoms are in the first column of the periodic table and hence they have a single valence electron, obviously the total spin of the atom depends on the nuclear spin, because the total spin of the atom is the sum of the nuclear spin and the outer electron spin. Therefore, they can be used to produce a gas with a resulting integer total spin, which means a gas of Bose particles [1]. However, this will lead to a gas with different types of

[1] As shown by Pauli; relativistic quantum field theory requires that particles with integer spin obey Bose, and particles with half-odd integer spin obey Fermi-Dirac statistics

bosons since the addition of two spins S_1 and S_2 leads to the possible different values of the total spin; $S = \mid S_1 - S_2 \mid, ..., S_1 + S_2$. After splitting the energy states, when the thermal equilibrium is reached, all the particles will settle to the ground state. Moreover, it is possible to construct a magneto optical trap (MOT) by producing a region of space in which the magnetic field has a local minimum, which serves as a local minimum in potential energy for the bosons. Therefore, atoms which are too energetic can escape from the trap, while cold atoms, which have less kinetic energy, will be bound by this local minimum.This can be viewed as cooling by evaporation. The cooling rate and the final temperature of the system can be controlled by changing the barrier height. One of the most important features of these trapped Bose gases is that they are inhomogeneous and therefore confined in space and BEC can be observed not only in momentum space but also in real space for these novel systems providing a feasible lab for interesting experimental studies.

3.2 BEC Theory

Bose (1924) and Einstein (1925) predicted that, below a certain temperature, a gas of noninteracting bosonic atoms will suddenly develop a macroscopic population in the ground state, which is called Bose-Einstein condensation

(**BEC**). It is easy to show how this prediction was made by analyzing the behavior of an ideal gas of N boson particles. If the volume of the gas is V, with periodic boundary conditions, any individual atom will be in a plane wave state with the periodic boundary conditions given by;

$$\psi(\mathbf{r}) = \frac{1}{V^{1/2}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

and k's are defined by L_x, L_y, L_z are the lengths of the parallelepiped volume in each direction,

$$\mathbf{k} = (\frac{2\pi n_x}{L_x}, \frac{2\pi n_y}{L_y}, \frac{2\pi n_z}{L_z})$$

and therefore volume is given by $V = L_x L_y L_z$, and $n_\alpha (\alpha = x, y, z)$ are integers.

For the particle with mass, m, the energy of each of these single particle quantum states is;

$$\epsilon_k = \frac{\hbar^2 k^2}{2m}$$

As a result, in momentum space, the number of single particle states in a thin shell between k_s and $k_s + \delta k_s$ can be written as;

$$M_s = 4\pi k_s^2 \delta k_s \frac{V}{(2\pi)^3}$$

The number of ways that N_s identical bose, i.e. indistinguishable, particles can be distributed in M_s available quantum states, can be given by the usual formula;

$$W_s = \frac{(N_s + M_s - 1)!}{N_s!(M_s - 1)!}$$

This number of available states in a given shell in momentum space gives the total number of available states for the whole gas as;

$$W = \prod_{\mathrm{s}} W_s = \prod_{\mathrm{s}} \frac{(N_s + M_s - 1)!}{N_s!(M_s - 1)!}$$

Here one can assume that $N_s, M_s \gg 1$, then the entropy of the gas can be written by using the Stirling's approximation, $lnN! \sim NlnN - N$, as ;

$$S = k_B \ln W = k_B \sum_s [(N_s + M_s) \ln(N_s + M_s) - N_s \ln N_s - M_s \ln M_s]$$

where k_B is the Boltzmann constant. In thermal equilibrium, for a fixed N and U, the entropy is maximized which means the equation to be solved is;

$$\frac{\partial S}{\partial N_s} - k_B\beta\frac{\partial U}{\partial N_s} + k_B\beta\mu\frac{\partial N}{\partial N_s} = 0$$

where $k_B\beta$ and $k_B\beta\mu$ are Lagrange multiplier constants, $\beta = 1/k_BT$, and μ is the chemical potential giving us;

$$\ln(N_s + M_s) - \ln N_s - \beta\epsilon_s + \beta\mu = 0$$

which can be rearranged to give;

$$N_s = \frac{1}{e^{\beta(\epsilon_s - \mu)} - 1} M_s$$

Therefore, one can write the average occupation number of any single particle state s as;

$$f_{BE}(\epsilon) = \frac{N_s}{M_s} = \frac{1}{e^{\beta(\epsilon_s - \mu)} - 1}$$

which is called Bose-Einstein distribution. By using this distribution the total number of particles in the volume can be rewritten;

$$N = \sum_k \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1}$$

From this expression for given N, the chemical potential can be determined. In the thermodynamic limit, where $V \to \infty$, one can turn the summation into integral and write;

$$N = \frac{V}{(2\pi)^3} \int \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1} d^3k$$

which gives the particle density as;

$$n = \frac{1}{(2\pi)^3} \int \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1} d^3k$$

Moreover one can use the density of states per unit volume, $g(\epsilon)$ to write the integral equation to define the particle density as a function of chemical potential and the temperature ;

$$n = \int_0^\infty \frac{1}{e^{\beta(\epsilon - \mu)} - 1} g(\epsilon) d\epsilon$$

Defining the dimensionless variables $z = e^{\beta\mu}$, which is called fugacity, and $x = \beta\epsilon$, we can rewrite this integral as;

$$n = \frac{(mk_BT)^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int\limits_0^\infty \frac{ze^{-x}}{1-ze^{-x}}x^{1/2}dx$$

The term in the integral can be simplified by using the expansion:

$$\frac{ze^{-x}}{1-ze^{-x}} = ze^{-x}(1 + ze^{-x} + z^2e^{-2x} + ...) = \sum_{p=1}^{\infty} z^p e^{-px}$$

which is convergent for $z < 1$, and the simplified integral will have the form :

$$\int\limits_0^\infty e^{-px}x^{1/2}dx = \frac{1}{p^{3/2}}\frac{\sqrt{\pi}}{2}$$

Using this result and defining the function $g_{3/2}(z) = \sum\limits_{p=1}^{\infty}\frac{z^p}{p^{3/2}}$, the particle density can be written as;

$$n = (\frac{mk_BT}{2\pi\hbar^2})^{3/2} g_{3/2}(z)$$

When the condensation occurs, majority of the bosons populate the ground state which yields the chemical potential(μ) to be zero and this point defines the critical temperature,T_c, for BEC;

$$T_c = \frac{2\pi\hbar^2}{mk_B}(\frac{n}{2.612})^{2/3}$$

where we have used $g_{3/2}(1) = 2.612$. We can write the total internal energy of the gas as;

$$U = V \int_0^\infty \frac{\epsilon}{e^{\beta(\epsilon-\mu)} - 1} g(\epsilon) d\epsilon$$

or, in terms of dimensionless variables we introduced before we can rewrite this as;

$$U = V \frac{(m)^{3/2}(k_B T)^{5/2}}{\sqrt{2}\pi^2\hbar^3} \int_0^\infty \frac{ze^{-x}}{1 - ze^{-x}} x^{3/2} dx$$

Then we can write the average energy per particle for $T > T_c$;

$$u = \frac{U}{N} = \frac{3}{2} k_B T \frac{g_{5/2}(z)}{g_{3/2}(z)}$$

and for $T < T_c$

$$u = \frac{U}{N} = \frac{3}{2} k_B \frac{T^{5/2}}{T_c^{3/2}} \frac{g_{5/2}(1)}{g_{3/2}(1)}$$

The heat capacity can be obtained by differentiating the internal energy while keeping the density constant, which gives us for $T \gg T_c$ $c_V \sim 3k_B/2$ and for $T < T_c$

$$c_V = \frac{15}{4} k_B \frac{g_{5/2}(1)}{g_{3/2}(1)} (\frac{T}{T_c})^{3/2}$$

In BEC state, below the critical temperature, T_c, normal gas particles and condensed particles coexist, but they are separated in momentum space in such a way that all the condensed particles occupy the zero momentum state, while the normal particles have finite momentum, and the heat capacity is proportional to $T^{3/2}$. Above T_c, all the particles are in normal state, and c_v

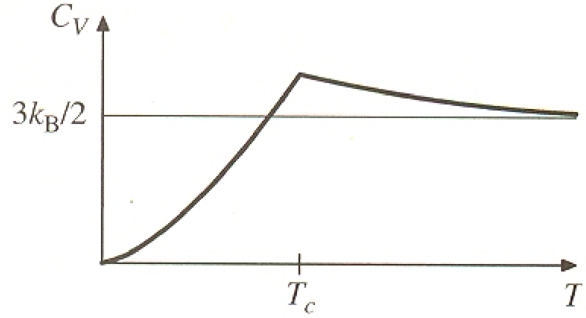

Figure 3.1: c_V vs T

approaches to its classical value of $3k_B/2$. This can be seen if we write the number of particles with energy $\epsilon > 0$ at $T < T_c$ with $\mu = 0$;

$$N_{\epsilon>0} = N\left(\frac{T}{T_C}\right)^{3/2}$$

and the number of particles with energy $\epsilon = 0$ is;

$$N_{\epsilon=0} = N\left(1 - (\frac{T}{T_C})^{3/2}\right)$$

Ehrenfest classified the phase transitions in terms of the derivative of free energy such that, at T_c if the first derivative shows discontinuity it is called first order, and if the second derivative of free energy is discontinuous then the transition is called second order. Although as it is written in J.F.Annett's book[4] that the BEC is usually interpreted as a first order phase transition, in the Statistical Physics book by L.D.Landau, and E.M.Lifshitz (page 170)[24], it is said that '*At the actual point $T = T_c$ all the thermody-*

namic quantities are mentioned (F, E, S, c_V) are continues. One can show, however, that the derivative of the specific heat with respect to temperature has a discontinuity at this point.' which makes BEC, according to Ehrenfest description, a second order phase transition.

3.3 ^{4}He

Although the superfluidity of ^{4}He was considered to be a manifestation of BEC at the time of its discovery, it didn't take too long to realize that the particle interactions in liquid ^{4}He are too strong to be neglected, hence the original theory of BEC had to be modified in order to describe it. Indeed, for noninteracting bosons the condensate fraction of particles is 100% at $T = 0$ while it is 10% for real ^{4}He due to the interactions. Therefore, the true BEC observation had to wait 70 years of improvement of experimental capabilities. Nowadays atomic BEC can be produced at temperatures of nano-Kelvin thanks to improved cooling techniques.

At 4^oK He becomes liquid and it's de Broglie wavelength is ≈0.4nm which is greater than the average interatomic distances ≈0.27nm which makes the quantum mechanical effects important. He doesn't have a solid phase for any temperature under 25 bars of pressure as can be seen in the phase diagram

Fig.3.2. Even though the gas-liquid phase transition line doesn't intersect the liquid-solid transition line, there is still a critical point for gas-liquid transition at 5.18^{o}K. It is also very unique having two different liquid phases (He-I and He-II). He-I is a normal liquid while He-II is a superfluid.

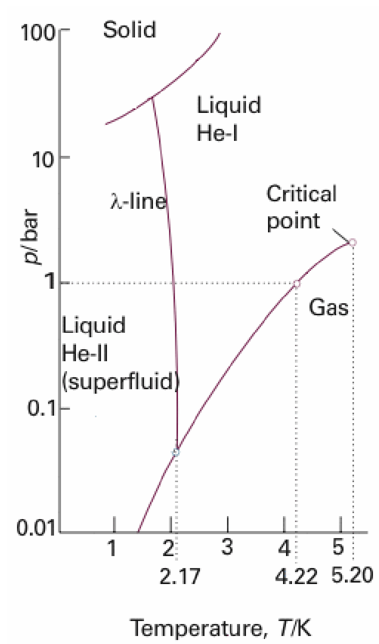

Figure 3.2: Phases of ^{4}He

Another unique property of helium is it's lambda shaped specific heat capacity graph Fig.3.3. One can compare the specific heat capacity of BEC (Fig.3.1) with this graph and see the completely different behavior at the T$_c$; while BEC has a simple change of slope, ^{4}He has much sharper feature. In order to explain the superfluidity of ^{4}He Landau worked out the Galilean

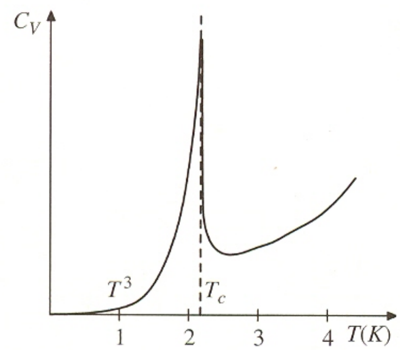

Figure 3.3: Specific heat capacity of ^{4}He

transformations of energy and momentum of the fluid. He wrote the energy and momentum in a reference system K' which moves with velocity V with respect to the reference system K as:

$$E' = E - \mathbf{P} \cdot \mathbf{V} + \frac{1}{2} M V^2 \tag{3.1}$$

and $\mathbf{P'} = \mathbf{P} - M\mathbf{V}$, where M is the total mass of the fluid.

If a viscous uniform fluid at $T = 0$ flows through a capillary at a constant velocity, v, then it's energy will be dissipated. Assuming that the dissipation occurs only because of the creation of excitations, one can write the energy of the system in the reference frame in which the capillary is stationary(apparently this reference frame moves with -v with respect to the fluid) with a single excitation of momentum p as:

$$E' = E_0 + \epsilon(p) + \mathbf{p} \cdot \mathbf{v} + \frac{1}{2} M v^2 \tag{3.2}$$

where E_0 is the ground state energy. Here, $\epsilon(p) + \mathbf{p} \cdot \mathbf{v}$ and $\mathbf{p}$ is the change in energy and momentum due to the appearance of the excitation respectively. An excitation can appear spontaneously only if $\epsilon(p) + \mathbf{p} \cdot \mathbf{v} < 0$ which gives us the condition $v > \frac{\epsilon(p)}{p}$ in which case the fluid is unstable and lose energy. On the other hand, if $v < v_c = min(p)\frac{\epsilon(p)}{p}$, then the previous condition is not going to be satisfied and no excitation will be created spontaneously, therefore v_c is the critical velocity below which the superfluidity is observed. It is important to note that the weakly interacting Bose gas fulfills the Landau's criterion with the critical velocity given by the velocity of sound, and the strongly interacting ^{4}He satisfies the Landau's criterion with a smaller critical velocity due to it's complicated excitation spectrum. However, because the ideal Bose gas can undergo Bose-Einstein condensation, it doesn't show superfluid behavior since its critical velocity is zero, and superfluidity needs interactions. Superfluidity without BEC can be observed in lower dimensions (1D, 2D)[35–37]. In 3D, condensation and superfluidity occur together. Landau also showed that the behavior of a uniform fluid at $T \approx 0$(small but nonzero) can be approximated to a gas of noninteracting excitations (quasiparticles) in thermal equilibrium. The quasiparticles can transport some part of the mass without creating new excitations which corresponds to a superfluid part of the system, and additional mass flow creates new excitations which then collide with the walls of the capillary. This results in dissipation of energy in the system which corresponds to normal flow. Therefore at low temperatures some part of the fluid behaves as a superfluid and the rest behaves as a viscous, "normal" liquid. The equilibrium velocity of the viscous fluid, v_n, is equal to the velocity of the frame where the capillary is at rest. Thus the relative velocity of superfluid and normal liquid is $v_s - v_n$, and the energy of the excitations in the capillary frame is given by $\epsilon(p) - \mathbf{p} \cdot (\mathbf{v_s} - \mathbf{v_n})$ in the reference frame where the superfluid is at rest. As a result, the equilibrium distribution of excitations is given by:

$$N_p = \frac{1}{\exp\left(\frac{\epsilon(p) - \mathbf{p}\cdot(\mathbf{v_s} - \mathbf{v_n})}{kT}\right) - 1} \tag{3.3}$$

If $v_s - v_n < v_c$, then this distribution function will be positive for all values of $\mathbf{p}$ which means that there is an equilibrium state in which there is no friction between the superfluid and normal component of the liquid.

Chapter 4

BCS-BEC Crossover

4.1 Historical Overview

The history of the relation between BEC and BCS theories is a long and complicated one. Before the BCS theory, since there are many similarities between fermi and bose superfluids, the superconductivity in metals was tried to be explained by BEC theory. The macroscopic occupation of a single quantum state is the basis for all bulk superfluids, and the off-diagonal long range order (ODLRO) is a unifying concept in the study of these two types of superfluids [38]. However, after the BCS theory was introduced, it didn't take long for researchers to point out the differences between BCS and BEC; namely the Cooper pairs are not composite bosons, the pairs are highly overlapping in real space and therefore they should be taken as momentum space pairs rather than real space, and also in BCS the current carriers are charged, Q=2e, while in BEC (^{4}He and atoms) charge is Q=0. However, in 1969, Eagles [3] showed that in the limit of very high densities using the BCS wave function to describe the fermion pairs which can become smaller than the interparticle distance, the pairs should be better described by Bose-Einstein statistics. The details of this theory was discussed by Leggett [1] and many others later on [2, 39] etc. Ultra cold atomic gases have unique features which enable experimentalists to work on different aspects of the interacting fermions and bosons. It is already known that Cooper pairs are formed between fermions below a critical temperature, but what happens when the interaction energy of the Cooper pair state is increased until it is close to the fermi energy is a question which is still under investigation. The proposed theories were mainly stating that the diatomic molecules (being composite bosons) would undergo BEC, and later on this was observed by many experimental groups (JILA, Innsbruck, MIT, Rice, ENS, Duke) the first of which was performed at JILA in 2003 [13]. In these experiments it was shown that as the interaction between fermionic atoms (such as K, Li, Rb) increased with the help of Feshbach resonances, a continual change from a BCS state of Cooper pairs to BEC state of diatomic molecules occurs, which is called *BCS-BEC crossover*, see Fig4.1. On the BCS side of the crossover the size of the fermion pairs is much larger than the interparticle distance while on the BEC side the size of the diatomic molecules is much smaller than the interparticle distance, and in the middle as the magnetic field strength is changed the size of the pairs changes smoothly from one limit to the other. Since the BCS-BEC crossover has been experimentally realized [12, 40, 41], ultracold neutral alkali atoms gases have become a new lab not only in condensed matter physics and atomic physics but there is "carry over " of physics to nuclear physics and hadron physics [42–44, 62].

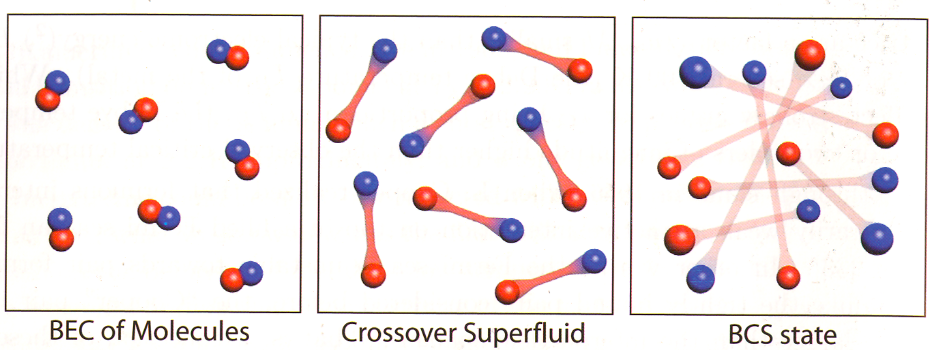

Figure 4.1: The BEC-BCS crossover: By tuning the interaction strength between two fermionic spin states, the size of fermion pairs can be changed from the small size of a molecular bound state in the BEC limit to the much larger size of long-range Cooper pairs compared to the interparticle spacing in the BCS limit. In the crossover regime the pair size is comparable to the interparticle spacing. While the size of the pair changes, the pair binding energy varies from the large binding energy of a molecule in the BEC limit to the small BCS value respectively[5].

4.2 Review of some Theory of Crossover

After the first discussion of crossover between BCS and BEC by Eagles[3], Leggett [1] proved that there is a smooth crossover from BCS ground state of Cooper pairs to a BEC of tightly bound diatomic molecules at $T = 0$ in dilute fermi gases. Later on Nozieres and Schmitt-Rink[2] showed that it might be possible to obtain this crossover by varying the density of carriers at $T \neq 0$. Several models interpolate between these two limits and describe the weak attraction, high density limit with BCS theory and the strong coupling, low density limit with the BEC theory.

In ultracold atomic fermions, by means of changing the sign and the magnitude of pairing interactions which can be controlled by the magnetically-tuned Fano-Feshbach resonances[45, 46] (see Appendix), one can drive the system from BCS to BEC type superfluidity. Feshbach resonances occur when the energy of scattering (open channel) between two particles and the energy of a bound state (closed channel) become close to each other. If the magnetic moments of the pairs of atoms are different in these two channels, then we can change the relative positions of energy curves by tuning the external magnetic field, and we can go from a situation in which the energy of the bound state is just below the threshold of the continuum to a situation where the same bound state is just above the threshold. The transition between two situations occurs at a particular value of the magnetic field, see Fig.4.2.

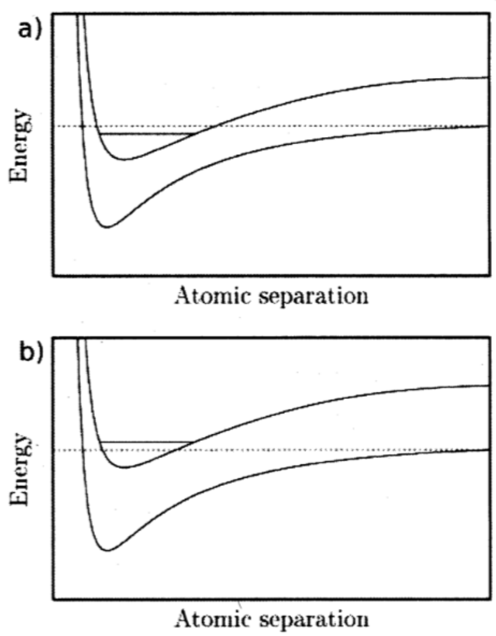

Figure 4.2: Fano-Feshbach resonance mechanism: The lower curve shows the scattering potential between two atoms in a given spin state(open channel), and the upper curve shows the interaction potential in different spin state(closed channel). The position of the bound state can be changed by changing the external magnetic field, and it can be moved from just below to just above the continuum excitations [6]

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Two-Body Collisions

For quantum degenerate dilute fermi gases the antisymmetry constraint of the wavefunction imposes that only particles with different spin can interact and their collisions are described by s-wave scattering length “a”. Neglecting the relativistic spin interactions, description of the collision process can be as simple as solving the Schrödinger equation:

$$\left(-\frac{\hbar^2}{2m_r}\nabla^2 + V(r) - \epsilon\right)\psi(r) = 0 \tag{4.1}$$

where $r = r_1 - r_2$ and $m_r = m_1 + m_2/(m_1 m_2)$ and V(r) is the interatomic potential whose range is fixed by R_0 . Once this equation is written in spherical polar coordinates the solution for positive energy, $\epsilon > 0$ in the region $r \gg R_0$ where $V(r) \approx 0$ can be given as:

$$\psi(r) \propto e^{i\mathbf{k}\cdot\mathbf{r}} + f(k,\theta)\frac{e^{ikr}}{r} \tag{4.2}$$

where $k = \sqrt{2m_r\epsilon}/\hbar$, θ is the angle between $\mathbf{k}$ and $\mathbf{r}$, and f is the scattering amplitude. When $k \to$0, f becomes independent of k and θ;

f($k \to$0,θ)= -a. Here, ”a” is the s-wave scattering length and it is the important parameter for describing the low energy scattering processes.

The scattering length for a given V(r) the wavefunction should be expanded into angular r or l-wave components and eq.4.1 must be solved for $l = 0$ which can be written as $\psi_0(r) = \chi_0(r)/r$, then with this at hand we can rewrite the Schrödinger equation as:

$$\frac{d^2\chi_0}{dr^2} + \frac{2m_r}{\hbar^2}[\epsilon - V(r)]\chi_0 = 0 \tag{4.3}$$

The solution of this equation for $r \gg R_0$ is $\chi_0 \propto sin[kr + \delta_0(k)]$ which can be used to write s-wave scattering length in terms of the phase shift $\delta_0(k)$;

$$f_0(k) = \frac{e^{2i\delta_0(k)} - 1}{2ik} = \frac{1}{kcot\delta_0(k) - ik} \tag{4.4}$$

The two-body bound states in the s-wave channel can be described by the solutions of eq.4.3 for $\epsilon < 0$ for $r \gg R_0$ which has the form;

$$\psi_b(r) \propto \frac{e^{-\sqrt{m_r|\epsilon_b|}r/\hbar}}{r} \tag{4.5}$$

where ϵ_b is the binding energy. For small ϵ_b values we should have the same result as for the $k \to 0$ which implies that bound states exists only for $a > 0$ and the binding energy is given as:

$$\epsilon_b = -\frac{\hbar^2}{2m_r a^2} \tag{4.6}$$

Notice that as $a \to \infty$ the binding energy vanishes and the scattering amplitude obeys the universal law $f_0 = i/k$, independent of the interactions which is called "unitarity limit". The fermionic interactions are strongest at the unitarity limit causing them to turn into diatomic molecules. Since the interaction strength is described by the s-wave scattering length a, at this limit a is longer than the interparticle distance. Fig.4.3 shows the results of some calculations for the gap Δ and the chemical potential μ at $T = 0$[7].

In the many body treatment of interactions one can use an effective poten-

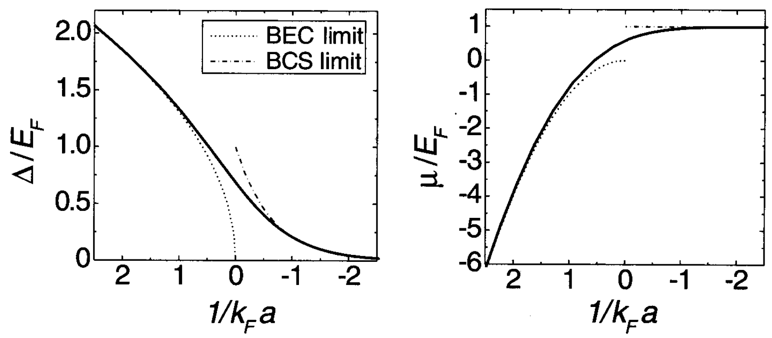

Figure 4.3: Gap parameter(Δ) and the chemical potential(μ) of a homogeneous Fermi gas at $T = 0$ (the solid line is the NSR theory calculations and dashed lines are the BCS and BEC limits of the theory). The unitarity limit is where the dimensionless parameter $1/k_F a \rightarrow 0$ [7]

tial V_{eff} since the low energy processes are independent of the details of the interactions. A regularized zero-range pseudo-potential defined by Huang and Yang in 1957[47] with a differential operator;

$$V_{eff}(r) = g\delta(r)\frac{\partial}{\partial r}r \tag{4.7}$$

where g is the coupling constant and given as $g = 2\pi\hbar^2 a/m_r$.This effective potential has a zero range, $R_0 = 0$ and therefore it acts only on s-wave component of the wavefunction. For $a > 0$ the bound state wavefunction can be solved by using pseudo-potential given in eq.4.7 and Schrödinger equation:

$$\psi_b = \frac{1}{\sqrt{2\pi a}}\frac{e^{-r/a}}{r} \tag{4.8}$$

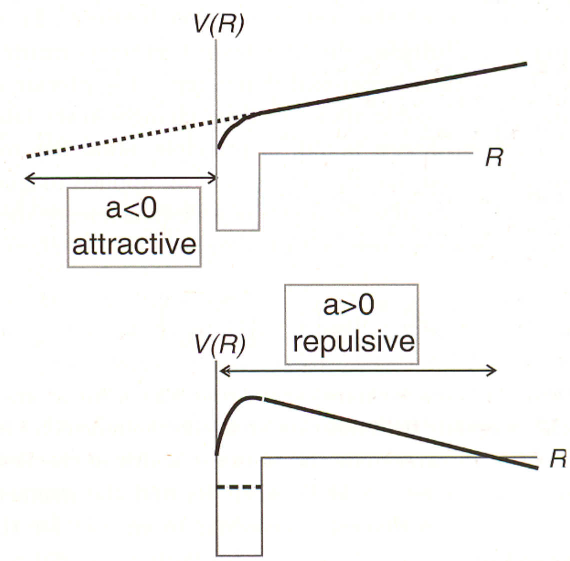

Figure 4.4: Top figure shows the scattering wave function when there is a deep attractive potential, and bottom figure shows when there is a deeper attractive potential where the bound state potential (dashed line) is near the threshold. R is the relative position of two fermions. The scattering length changes sign as the bound state energy changes through Feshbach resonance. The sign of the scattering length decides whether the effective interaction will be attractive(a<0) or repulsive(a>0)[7]

4.3 Review of the Experiments

The first Bose-Einstein Condensation(BEC) was realized in 1995 [32–34] in dilute vapors of alkali atoms. This discovery triggered a huge amount of experimental and theoretical work in the area. At first, the researchers were concentrated on the consequences of BEC, therefore studies were done with bosonic gases. Later on the Fermi gases started to get attention, because from the many-body point of view Fermi superfluidity has richer physics.

The first degenerate Fermi gas of atoms was created by B. DeMarco and D. Jin in 1999 at JILA by using fermionic ^{40}K[48]. In 2002 Feshbach resonances started to play an important role in experiments and in 2003 the first Feshbach molecules were observed [49]. In these experiments, by sweeping the magnetic field across the Feshbach resonance, they tuned the energy of the Feshbach molecular state below that of two free atoms, and therefore molecules could be produced, and it didn't take too long to cool down the molecules consisting of pairs of fermionic atoms into BEC [13, 40, 41], and the first direct observation of BEC was made in 2004 [50]. All these experiments were in the strongly interacting regime with $k_F a > 1$, where the size of the pairs is comparable to the interparticle spacing. Therefore, these experiments were already realizing the crossover condensates. Within months, the observation of fermion pair condensation was extended throughout the whole BCS-BEC crossover region [11, 12]. Experiments during the following years were mostly concentrated on the thermodynamic measurements of this new crossover superfluid. Finally, in 2005 superfluidity and phase coherence was directly demonstrated with the observation of vortices [8], see Fig.4.5

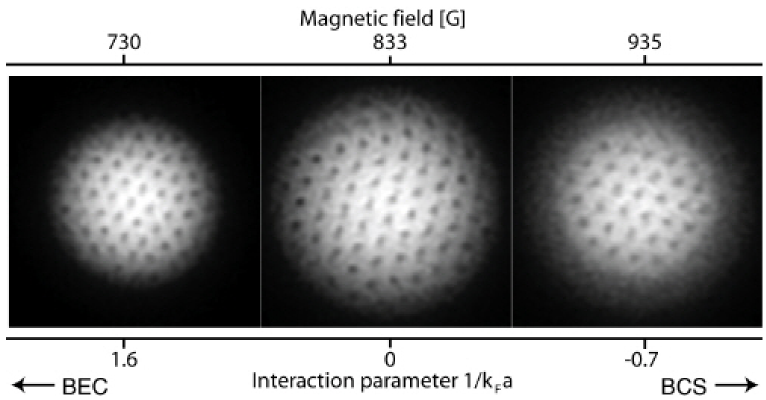

Figure 4.5: Vortices throughout the BCS-BEC crossover in a gas of ^{6}Li[8]

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4.4 Comparison with other superfluids

This new type of superfluid differs from ^{3}He, conventional and high-T$_c$ superconductors in its high critical temperature with respect to the Fermi temperature as can be seen in Table- 4.4, $T_c/T_F \approx 0.2$ and this is the reason for these systems to be called *high-temperature superfluidity*. However, the crossover and high-T$_c$ problems shares several features; while in the crossover regime the pair size is comparable to interparticle spacing, in high-T$_c$ superconductors the correlation length is comparable to the distance between electrons, therefore both systems are composed of strongly correlated fermions, and in both cases above the phase transition temperature correlations are still strong enough to form uncondensed pairs at finite momentum.

System	T_c	T_F	$T_c\ /T_F$
Conventional superconductors	1-10K	(0.5-1.5)$\cdot 10^5$K	$10^{-4} - 10^{-5}$
^{3}He	0.0026K	5K	0.0005
High-T_c superconductors	35-140 K	2000-5000K	0.01-0.05
Strongly interacting atomic Fermi gases	0.2μK	1μK	0.2

Table-4.4 The critical temperature with respect to Fermi temperature for different systems.

Interactions between ultracold atoms are described by $g = 2\pi\hbar^2 a/m_r$ which is fixed by the exact s-wave scattering length a. For identical fermions, there is no s-wave scattering due to Pauli-principle. In the regime ka$_c$ <<1 where $a_c = (2m_r C_6/\hbar^2)^{1/4}$ is the Van der Waals length, all the higher momenta ($l \neq 0$) are frozen out, and a single component fermi gas approaches an ideal , non-interacting quantum gas. For identical fermions, p-wave collisions at low temperatures has vanishing scattering rates ($\approx T^2$) which makes it impossible to use evaporative cooling techniques.

In the case of mixtures of fermions in different internal states (or for bosons) there is in general a finite scattering length (a $\neq$ 0), which is typically in the order of the Van der Waals length. Interactions are weak when the scattering length is much smaller than the average interparticle spacing. Since the ultracold alkali gases have densities between 10^{12}-10^{15} particles per cm^3, the average interparticle spacing ($n^{-1/3}$) is in the range 0.1-1μm, and the scattering lengths is in few nm range, therefore the interaction effects are mostly negligible. However in the attractive case (a<0), even small interactions can cause instabilities. Specifically speaking attractive bosons are unstable towards BEC.

Chapter 5

The Macroscopic Coherent State

5.1 Coherent States

Coherent states were first proposed by Schrödinger right after the birth of quantum mechanics in 1926, but important applications were made by Glauber [51], Klauder[52, 53], and Sudarshan[54] in 1963 to quantum optics. The term *coherent state* was first used by Glauber. In order to describe the quantized electromagnetic radiation field, he constructed the eigenstates of the annihilation operator of the harmonic oscillator. The complete construction of coherent states of any Lie group was achieved in 1972 by Perelomov and Gilmore[55, 56]. As was stated by Glauber there are three different (but equivalent) ways to define the field coherent states of a dynamical group of the system:

Definition − 1: The coherent states are eigenstates of the lowering operator (of the harmonic oscillator):

$$\hat{c}\,|\alpha\rangle = \alpha\,|\alpha\rangle \tag{5.1}$$

and

$$\langle\alpha|\,\hat{c}^{\dagger} = \langle\alpha|\,\alpha^{*} \tag{5.2}$$

where α is complex, and $\hat{c}, \hat{c}^{\dagger}$ are bosonic annihilation and creation operators and they obey the commutation relation; $[\hat{c}, \hat{c}^{\dagger}] = 1$. Even though it seems easy to use this definition, it has major problems. With this definition the eigenvalue equations are non-Hermitian and the eigenvalues are complex, and the coherent states can't be defined in finite dimensional Hilbert spaces. Moreover, the only physically realizable 'Glauber' coherent states are the electromagnetic field states since this is the only system with $\hat{c}$ and $\hat{c}^{\dagger}$ are both the multiple of the identity operator. Therefore this first definition is not widely applicable.

Definition − 2: The coherent states are quantum states with a minimum uncertainty.

$$(\Delta p)^2(\Delta q)^2 = (\frac{1}{2})^2 \tag{5.3}$$

where p and q are defined by:

$$\hat{p} = \frac{1}{i\sqrt{2}}(\hat{c} - \hat{c}^{\dagger}) \tag{5.4}$$

$$\hat{q} = \frac{1}{\sqrt{2}}(\hat{c} + \hat{c}^{\dagger}) \tag{5.5}$$

Apparently these equations can't provide unique solutions for p and q. Such coherent states are known as 'intelligent' states in the literature. These coherent states can only be constructed for classically integrable systems, and this condition reduces the commutation relations to those of photon creation and annihilation operators. Moreover, different wave packets with minimum uncertainty may have different properties, and they may be incomplete.

Definition – 3: The coherent states can be constructed by the application of a displacement operator on a reference state $|\zeta\rangle$.

$$|\alpha\rangle = D(\alpha)\,|\zeta\rangle \tag{5.6}$$

where $D(\alpha) = exp(\alpha\hat{c}^{\dagger} - \alpha^{*}\hat{c})$ is the displacement operator.

Here it is important to note that the choice of the reference state is in principle arbitrary, but for a specific dynamic system, construction of a useful coherent states depends on this choice since the reference state will determine the structure of the coherent states as well as the structure of the phase space of the system. Annett[4] used this definition to write down a coherent state:

$$|\alpha\rangle = e^{-|\alpha|^2/2} exp(\alpha\hat{c}^{\dagger})\,|0\rangle \tag{5.7}$$

where $|0\rangle$ is the ground state.

5.2 Coherent State of BCS

The BCS theory states that the superconducting current is a superfluid of Cooper pairs, i.e. *pairs of electrons* interacting through the exchange of phonons, therefore one can rewrite the BCS Hamiltonian in a more convenient way to introduce the coherent states.

The BCS Hamiltonian is given by;

$$H_{BCS} = \sum_{k} \varepsilon_k a_k^{\dagger} a_k + g \sum_{k,k'} a_k^{\dagger} a_{-k}^{\dagger} a_{-k'} a_{k'} \tag{5.8}$$

where $a_k^{\dagger}$ and a_k are the fermionic creation and annihilation operators satisfying the anticommutation relation;

$$[a_k^{\dagger}, a_{k'}]_+ = \delta(k, k') \tag{5.9}$$

and $\varepsilon_k = \hbar^2 k^2/2m - \mu$.

Here one can define J operators as:

$$J_{1k} = \frac{-1}{2}(a_k^{\dagger} a_{-k}^{\dagger} + a_{-k} a_k) \tag{5.10}$$

$$J_{2k} = \frac{i}{2}(a_k^{\dagger} a_{-k}^{\dagger} - a_{-k} a_k) \tag{5.11}$$

$$J_{3k} = \frac{-1}{2}(1 - a_k^{\dagger} a_k - a_{-k}^{\dagger} a_{-k}) \tag{5.12}$$

With these definitions J operators are the generators of SU(2) algebra satisfying the commutation rules:

$$[J_{pk}, J_{qk}] = i\epsilon_{pqr}J_{rk} \tag{5.13}$$

where (p,q,r)=(1,2,3)

and we can define J^+ and J^- operators as;

$$J_k^+ = -J_{1k} - iJ_{2k} \tag{5.14}$$

$$J_k^- = -J_{1k} + iJ_{2k} \tag{5.15}$$

where

$$[J_k^+, J_k^-] = 2J_{3k} \tag{5.16}$$

With these definitions we can rewrite the Hamiltonian as;

$$H_{BCS} = \sum_k (2\varepsilon_k J_{3k} + 4\Delta_k J_{1k}) \tag{5.17}$$

Here the first term is the kinetic energy, $\sum_k 2\varepsilon_k J_{3k}$ and the second term is the interaction energy, $\sum_k 4\Delta_k J_{1k}$, where eq.2.61 defines the gap parameter (Δ_k). Yosida[57] gave the BCS coherent state for an isolated k as;

$$|\phi^0_{BCS}\rangle = e^{iS_f}\,|vacuum\rangle = e^{\theta_k(J_k^+ - J_k^-)}\,|vacuum\rangle \tag{5.18}$$

where S_f is given by;

$$S_f = -i\theta_k^f (J_k^+ - J_k^-) \tag{5.19}$$

The expectation value of $\hat{H}$ in the ground state is;

$$\langle \phi_{BCS}^0 | H_{BCS} | \phi_{BCS}^0 \rangle = \langle vacuum | e^{-iS_f} H_{BCS} e^{iS_f} | vacuum \rangle \tag{5.20}$$

We can say that the term between the vacuum states is the similarity transformation of Hamiltonian which diagonalizes it;

$$H'_{BCS} = e^{-iS_f} H_{BCS} e^{iS_f} \tag{5.21}$$

and using the Baker-Hausdorff Lemma we can calculate H'_{BCS} for an isolated k as;

$$H'_{BCS} = [2\varepsilon_k cos2\theta_k^f + 4\Delta_k sin2\theta_k^f] J_{3k} + [-2\varepsilon_k sin2\theta_k^f + 4\Delta_k cos2\theta_k^f] J_{1k} \tag{5.22}$$

here the usual diagonalization of the Hamiltonian can be done by equating the coefficient of J_{1k} to zero which gives the usual gap parameter as:

$$tan2\theta_k^f = \frac{2\Delta_k}{\varepsilon_k} \tag{5.23}$$

And now we can calculate the expectation value easily by writing;

$$\begin{aligned} \langle \phi_{BCS}^0 | H_{BCS} | \phi_{BCS}^0 \rangle &= \langle vacuum | H'_{BCS} | vacuum \rangle \\ &= [2\varepsilon_k cos2\theta_k^f + 4\Delta_k sin2\theta_k^f] \langle vacuum | J_{3k} | vacuum \rangle \\ &+ [-2\varepsilon_k sin2\theta_k^f + 4\Delta_k cos2\theta_k^f] \langle vacuum | J_{1k} | vacuum \rangle \end{aligned} \tag{5.24}$$

and finding the vacuum expectation values of J_{3k} and J_{1k} as;

$$\begin{aligned}\langle vacuum| J_{3k} |vacuum\rangle &= \langle vacuum| 1/2(n_k + n_{-k} - 1) |vacuum\rangle \\ &= 1/2(n_k^0 + n_{-k}^0 - 1)\end{aligned} \quad (5.25)$$

where $n_k = a_k^\dagger a_k$ and $n_{-k} = a_{-k}^\dagger a_{-k}$

$$\langle vacuum| J_{1k} |vacuum\rangle = \langle vacuum| (-1/2)(J_k^+ + J_k^-) |vacuum\rangle = 0 \quad (5.26)$$

gives the ground state expectation value of our transformed Hamiltonian as;

$$\langle \phi_{BCS}^0| H_{BCS} |\phi_{BCS}^0\rangle = (1/2)(n_k^0 + n_{-k}^0 - 1)[2\varepsilon_k cos2\theta_k^f + 4\Delta_k sin2\theta_k^f] \quad (5.27)$$

5.3 Coherent State of BEC

bosons are defined as particles with integer spin. Alkali atoms are in the first column of the periodic table and they have a single valence electron. So the total spin of the atom depends on the nuclear spin, since the total spin of the atom is the sum of the nuclear spin and the valence electron spin. We can produce a gas with a resulting integer total spin, which means we have a gas of Bose particles[4].

A simple Hamiltonian of a many boson system has been taken as[58];

$$H_{BEC} = \sum_k [\epsilon_k (c_k^\dagger c_k + c_{-k}^\dagger c_{-k} + 1) + V(c_k^\dagger c_{-k}^\dagger + c_{-k} c_k)] \quad (5.28)$$

where $c_k^\dagger$ and c_k are the creation and annihilation operator for bosons and they satisfy the commutation relation;

$$[c_k^\dagger, c_{k'}]_- = \delta_{k,k'} \tag{5.29}$$

Note that this is the same commutation relation as for harmonic oscillator.

From the above we can define K operators which obey SU(1,1) algebra as;

$$K_{1k} = (-1/2)(c_k^\dagger c_{-k}^\dagger + c_{-k}c_k) \tag{5.30}$$

$$K_{2k} = (i/2)(c_k^\dagger c_{-k}^\dagger - c_{-k}c_k) \tag{5.31}$$

$$K_{3k} = (1/2)(c_k^\dagger c_k + c_{-k}^\dagger c_{-k} + 1) \tag{5.32}$$

These hermitian operators satisfy the commutation rules:

$$\begin{aligned} [K_{1k}, K_{2k}] &= -iK_{3k} \\ [K_{2k}, K_{3k}] &= iK_{1k} \\ [K_{3k}, K_{1k}] &= iK_{2k} \end{aligned} \tag{5.33}$$

$$K_k^+ = c_k^\dagger c_{-k}^\dagger \tag{5.34}$$

$$K_k^- = c_{-k}c_k \tag{5.35}$$

and

$$[K_k^+, K_k^-] = -2K_{3k} \tag{5.36}$$

So we can write the Hamiltonian in terms of K operators as;

$$H_{BEC} = \sum_k 2\epsilon_k K_{3k} - 2VK_{1k} \tag{5.37}$$

Here the first term is in the kinetic energy, $\sum_k 2K_{3k}$, and the second term is the interaction energy,$\sum_k -2VK_{1k}$. And the coherent state of a BEC system is given by Birman[59];

$$|\phi^0_{BEC}\rangle = e^{iS_b}\,|n\rangle_b = |n\rangle_\mu \tag{5.38}$$

where $|n\rangle_b$ is a boson number eigenstate, and

$$S_b = -i(\theta^b_k/2)(K^+_k - K^-_k) = i\theta^b_k K_{2k} \tag{5.39}$$

Note θ^b_k is a parameter for the coherent state.

If we write the expectation value of H we will read;

$$_\mu\langle n|\, H_{BEC}\, |n\rangle_\mu =_b \langle n|\, e^{-iS_b} H_{BEC} e^{iS_b}\, |n\rangle_b \tag{5.40}$$

and the center term is the diagonalized Hamiltonian of the system;

$$H'_{BEC} = e^{iS_b} H_{BEC} e^{-iS_b} = e^{(\theta^b_k/2)(K^+_k - K^-_k)} H_{BEC} e^{(-\theta^b_k/2)(K^+_k - K^-_k)} \tag{5.41}$$

By using Baker-Hausdorff Lemma which is given as;

$$e^{iG\lambda} A e^{-iG\lambda} = A + i\lambda[G,A] + (i\lambda)^2/2![G,[G,A]] + ... \tag{5.42}$$

We can write the transformed Hamiltonian for one single k as;

$$H'_{BEC} = 2K_3(\epsilon_k cosh\theta^b_k - V sinh\theta^b_k) + 2K_1(\epsilon_k sinh\theta^b_k - V cosh\theta^b_k) \tag{5.43}$$

So the expectation value of this Hamiltonian is;

$$
\begin{aligned}
{}_b\langle n|\, H'_{BEC}\, |n\rangle_b = \\
2(\epsilon_k cosh\theta_k^b - V sinh\theta_k^b)_b \langle n|\, K_3\, |n\rangle_b \\
+2(\epsilon_k sinh\theta_k^b - V cosh\theta_k^b)_b \langle n|\, K_1\, |n\rangle_b
\end{aligned}
\tag{5.44}
$$

by finding the expectation values of K_1 and K_3

$$
{}_b\langle n|\, K_3\, |n\rangle_b ={}_b \langle n|\, ((1/2)(n_k + n_{-k} + 1)\, |n\rangle_b = (1/2)(n_k^0 + n_{-k}^0 + 1) \tag{5.45}
$$

$$
{}_b\langle n|\, K_1\, |n\rangle_b ={}_b \langle n|\, ((-1/2)(K_k^+ + K_k^-))\, |n\rangle_b = 0 \tag{5.46}
$$

Finally we can write the expectation value of our transformed Hamiltonian as;

$$
{}_\mu\langle n|\, H_{BEC}\, |n\rangle_\mu ={}_b \langle n|\, H'_{BEC}\, |n\rangle_b = 2(\epsilon_k cosh\theta_k^b - V sinh\theta_k^b)(1/2)(n_k^0 + n_{-k}^0 + 1) \tag{5.47}
$$

5.4 The Macroscopic Coherent State of BCS-BEC Crossover

Possible Interaction Terms for Crossover

In order to analyze a solvable model, there are several attractive possibilities for interactions. A 'minimal' model will preserve the known pure BCS and pure BEC Hamiltonians (mixture of bosons and fermions) and add a boson-fermion conversion (interaction) term. The Hamiltonian for our model is in that case;

$$H = H_{BCS} + H_{BEC} + H_{int} \tag{5.48}$$

with the eigenvalue equation;

$$H\left|k\right\rangle = E_k\left|k\right\rangle \tag{5.49}$$

Although throughout this research we have considered numerous possible interaction terms including;

$$H_{int} = \gamma_k(a_k^\dagger a_k c_k^\dagger c_k + a_{-k}^\dagger a_{-k} c_{-k}^\dagger c_{-k}) \tag{5.50}$$

and,

$$H_{int} = \gamma_k a_k^\dagger c_k + \gamma_k^* a_k c_k^\dagger \tag{5.51}$$

where $\hat{a}$ and $\hat{c}$ are annihilation operator for fermions and bosons respectively, we finally decided the interactions could be best described by the term;

$$H_{int} = \gamma_k(a_{-k} a_k c_0^\dagger + a_k^\dagger a_{-k}^\dagger c_0) \tag{5.52}$$

Because a Feshbach molecule is created from two fermions, and this term annihilates two fermions and creates a boson, or annihilates a boson and creates two fermions.

Finally with this choice of the interaction term, the meanfield Hamiltonian for BCS-BEC systems can be written as:

$$H = \sum_{p,p'}[\varepsilon_p(2J_{3p}+1) - V(J_p^+ J_{p'}^-)] + \sum_p [\Omega_p(2K_{3p} - \frac{1}{2}) + \frac{g_0}{2}(K_p^+ K_p^-)] + \sum_p [\gamma_p(c_0^\dagger J_p^- + c_0 J_p^+)] \tag{5.53}$$

Here the first term is the usual BCS Hamiltonian, the second is the usual BEC and the third is our choice for the interactions between molecules and atoms, $\varepsilon_p = \epsilon_p - \mu$ where ϵ_p stands for the kinetic energy of an atom and μ is the chemical potential, $V < 0$ is the atom-atom attraction potential and g_0 is the molecule-atom repulsion, and $\Omega_p = \frac{p^2}{2m} + 2\nu - 2\mu$ with ν being the threshold energy of the Feshbach resonance and γ_p is the atom-molecule coupling.

A trial Wavefunction

The SU(2) coherent state for a single particle is given as:

$$|\xi, j, m\rangle = T_f(\xi)\,|j,m\rangle = e^{(\xi J^+ - \xi^* J^-)}\,|j,m\rangle \tag{5.54}$$

where $\xi = \frac{\theta}{2}e^{-i\varphi}$, $\theta \in (0,\pi)$, $\varphi \in (0, 2\pi)$, and $|j,m\rangle$ is the eigenstate of J_3 with the eigenvalue of m (m=-j,-j+1,...,j-1,j). And the $J^\pm$ operators have the eigenvalue equations:

$$J^\pm\,|j,m\rangle = [(j \mp m)(j \pm m + 1)]^{1/2}\,|j, m \pm 1\rangle \tag{5.55}$$

And the SU(1,1) coherent state is given by:

$$|z, k, n\rangle = T_b(z)\,|k, n\rangle = e^{(zK^+ - z^*K^-)}\,|k, n\rangle \tag{5.56}$$

where $z = -\frac{\Theta}{2}e^{-i\phi}$, $\Theta \in (-\infty, \infty)$, $\phi \in (0, 2\pi)$, and $k > 0$ is the Bargmann index and the eigenvalue equations for $|k, n\rangle$ is:

$$K_{3,k}\,|k, n\rangle = (k+n)\,|k, n\rangle \tag{5.57}$$

$$K_k^+\,|k, n\rangle = [(n+1)(n+2k)]^{1/2}\,|k, n+1\rangle \tag{5.58}$$

$$K_k^-\,|k, n\rangle = [n(n+2k-1)]^{1/2}\,|k, n-1\rangle \tag{5.59}$$

Finally $D(\alpha)$ in the eq.5.61 is the displacement operator, $D^\dagger(\alpha)cD(\alpha) = c+\alpha$, and it is given by:

$$D(\alpha) = e^{(\alpha c^\dagger - \alpha^* c)} \tag{5.60}$$

where $\alpha = \langle\psi|\,c\,|\psi\rangle$, and $\alpha = |\alpha|e^{i\varphi_\alpha}$

We will follow Huang et al.[60] who showed that the coupled BCS-BEC systems are in generalized SU(2)$\otimes$ SU(1,1) coherent states which is given by:

$$|\psi\rangle = \left[\prod_p T_f(\xi_p)\,|j_p m_p\rangle\right] \otimes \left[D(\alpha)T_b(z_0)\,|k_0 n_0\rangle \prod_{p\neq 0} T_b(z_p)\,|k_p n_p\rangle\right] \tag{5.61}$$

where $j_p = k_p = \frac{1}{2}, k_0 = \frac{1}{4}, m_p = \pm\frac{1}{2}, n_p = 0, 1, 2, 3, ...$ and the normalization relation is given by:

$$\langle\psi|\psi\rangle = 1 \tag{5.62}$$

At $T = 0$ almost all molecules are in condensed state of $\mathbf{p}$=0, and for these molecules $c_k \to c$, where c is the annihilation operator for the ground state, and the pair operators can be written as:

$$K_{3,0} = \frac{1}{2}\left(c^\dagger c + \frac{1}{2}\right) \tag{5.63}$$

$$K_0^+ = \frac{1}{2}(c^\dagger)^2 \tag{5.64}$$

$$K_0^- = \frac{1}{2}c^2 \tag{5.65}$$

One can obtain the unitary transformations of the operators of Lie algebra by using Baker-Haussdorf formula:

$$T_b^\dagger(z_0)\hat{c}T_b(z_0) = cosh\left(\frac{\Theta_0}{2}\right)\hat{c} - e^{-i\phi_0}sinh\left(\frac{\Theta_0}{2}\right)\hat{c}^\dagger \tag{5.66}$$

$$T_b^\dagger(z_0)\hat{c}^\dagger T_b(z_0) = cosh\left(\frac{\Theta_0}{2}\right)\hat{c}^\dagger - e^{i\phi_0}sinh\left(\frac{\Theta_0}{2}\right)\hat{c} \tag{5.67}$$

and the similar relations hold for the $p \neq 0$ case. Similarly, for the fermionic single particle operators one can write:

$$T_f^\dagger(\xi_p)\hat{a}_{\pm p}T_f(\xi_p) = cos\left(\frac{\theta_p}{2}\right)\hat{a}_\pm \pm e^{-i\varphi_p}sin\left(\frac{\theta_p}{2}\right)\hat{a}^\dagger_{\mp p} \tag{5.68}$$

And for the pair operators:

$$T_b^\dagger \hat{K}^{\pm} T_b = cosh^2\left(\frac{\Theta}{2}\right)\hat{K}^{\pm} + e^{\pm 2i\phi} sinh^2\left(\frac{\Theta}{2}\right)\hat{K}^{\mp} - e^{\pm i\phi} sinh(\Theta)\hat{K}_3 \quad (5.69)$$

$$T_b^\dagger \hat{K}_3 T_b = cosh(\Theta)\hat{K}_3 - \frac{1}{2} sinh(\Theta)\left(e^{-i\phi}\hat{K}^{+} + e^{i\phi}\hat{K}^{-}\right) \quad (5.70)$$

$$T_f^\dagger \hat{J}^{\pm} T_f = cos^2\left(\frac{\theta}{2}\right)\hat{J}^{\pm} - e^{\pm 2i\varphi} sin^2\left(\frac{\theta}{2}\right)\hat{J}^{\mp} - e^{\pm i\varphi} sin(\theta)\hat{J}_3 \quad (5.71)$$

$$T_f^\dagger \hat{J}_3 T_f = cos(\theta)\hat{J}_3 + \frac{1}{2} sin(\theta)\left(e^{i\varphi}\hat{J}^{-} + e^{-i\varphi}\hat{J}^{+}\right) \quad (5.72)$$

With these transformed operators one can find the eigenvalue of the Hamiltonian as:

$$\begin{aligned} \langle H\rangle = &\sum_{p,p'}[\varepsilon_p(2\langle J_{3p}\rangle + 1) - V(\langle J_p^+\rangle\langle J_{p'}^-\rangle)] \\ &+ \sum_p[\Omega_p(2\langle K_{3p}\rangle - \frac{1}{2}) + \frac{g_0}{2}(\langle K_p^+\rangle\langle K_p^-\rangle)] \\ &+ \sum_p[\gamma_p(\langle c_0^\dagger\rangle\langle J_p^-\rangle + \langle c_0\rangle\langle J_p^+\rangle)] \end{aligned} \quad (5.73)$$

$$\begin{aligned} \langle H\rangle = &\sum_p[\varepsilon_p(2m_p cos\theta_p + 1)] + \sum_p[\langle J_p^+\rangle(-V\sum_{p'}\langle J_{p'}^-\rangle + \gamma_p\langle c_0\rangle)] \\ &+\Omega_0(2\langle K_{30}\rangle - \frac{1}{2}) + 2g_0(\langle K_0^+\rangle\langle K_0^-\rangle) \\ &+\sum_{p\neq 0}[\Omega_p(2\langle K_{3p}\rangle - \frac{1}{2}) + \frac{g_0}{2}(\langle K_p^+\rangle\langle K_p^-\rangle) + \frac{g_0}{2}(\langle K_0^+\rangle\langle K_p^-\rangle) + \frac{g_0}{2}(\langle K_p^+\rangle\langle K_0^-\rangle)] \\ &+\sum_p[\gamma_p(\langle c_0^\dagger\rangle\langle J_p^-\rangle)] \end{aligned} \quad (5.74)$$

here $\varepsilon_p = \epsilon_p - \mu_F; \epsilon_p = p^2/2m$, g_0 is molecule-molecule repulsion, $\Omega_p = E_p - \mu_B$; $E_p = p^2/4m + 2\nu$; ν is the threshold energy of FR and $\mu_F = \mu_B/2 = \mu$, γ_p is the atom-molecule coupling. Defining $(-V\sum_{p'}\langle J_{p'}^-\rangle) = \Delta_p$ and $(-V\sum_{p'}\langle J_{p'}^-\rangle + \gamma_p\langle c_0\rangle) = \tilde{\Delta}_p$ is the effective BCS gap function. Also $\langle c_0^\dagger\rangle = \alpha^*$ and $\langle c_0\rangle = \alpha$. Using these and the individual eigenvalues of the transformed operators one can rewrite the eigenvalue as:

$$\begin{aligned}
\langle H\rangle = \sum_p[\varepsilon_p(2m_p cos\theta_p + 1)] + \sum_p[-e^{i\varphi_p}m_p sin\theta_p\tilde{\Delta}_p] \\
+\sum_p[\gamma_p\alpha^*(-e^{-i\varphi_p}m_p sin\theta_p)] \\
+\Omega_0[\alpha^2 + 2(n_0+k_0)cosh\Theta_0 - \frac{1}{2}] \\
+\frac{g_0}{2}[(\alpha^2 - 2(n_0+k_0)sinh\Theta_0 e^{i\phi_0})(\alpha^2 - 2(n_0+k_0)sinh\Theta_0 e^{-i\phi_0})] \\
+\sum_{p\neq 0}[\Omega_p\left(2(n_p+k_p)cosh\Theta_p - \frac{1}{2}\right) \\
+\left(\frac{g_0}{2}\right)(-(n_p+k_p)sinh\Theta_p e^{i\phi_p})(-(n_p+k_p)sinh\Theta_p e^{-i\phi_p}) \\
+\left(\frac{g_0}{2}\right)\left(\frac{\alpha^2}{2} - (n_0+k_0)sinh\Theta_0 e^{i\phi_0}\right)\left(-(n_p+k_p)sinh\Theta_p e^{-i\phi_p}\right) \\
+\left(\frac{g_0}{2}\right)\left(-(n_p+k_p)sinh\Theta_p e^{i\phi_p}\right)\left(\frac{\alpha^2}{2} - (n_0+k_0)sinh\Theta_0 e^{-i\phi_0}\right)]
\end{aligned} \tag{5.75}$$

substitution of $m_p = -1/2$, $n_p = n_0 = 0$, $k_p = 1/2$ and $k_0 = 1/4$ reduces this expression to:

$$\langle H\rangle = \sum_p [\varepsilon_p(1-cos\theta_p) + \frac{1}{2}(e^{i\varphi_p}sin\theta_p\tilde{\Delta}_p) + \frac{1}{2}(\gamma_p\alpha^*(e^{-i\varphi_p}sin\theta_p))]$$
$$+\Omega_0[\alpha^2 + \frac{1}{2}(cosh\Theta_0 - 1)] + \frac{g_0}{2}[(\alpha^4 - \frac{\alpha^2}{2}sinh\Theta_0 cos\phi_0 + \frac{1}{4}sinh^2\Theta_0]$$
$$+\sum_{p\neq 0}[\Omega_p\left(cosh\Theta_p - \frac{1}{2}\right) + \frac{g_0}{2}\left(\frac{1}{4}sinh^2\Theta_p\right) \quad (5.76)$$
$$+\frac{g_0}{2}\left(\frac{\alpha^2}{2} - \frac{1}{4}sinh\Theta_0 e^{i\phi_0}\right)\left(-\frac{1}{2}sinh\Theta_p e^{-i\phi_p}\right)$$
$$+\left(\frac{g_0}{2}\right)\left(-\frac{1}{2}sinh\Theta_p e^{i\phi_p}\right)\left(\frac{\alpha^2}{2} - \frac{1}{4}sinh\Theta_0 e^{-i\phi_0}\right)]$$

For real α (i.e. $\varphi_\alpha = 0$) with $\varphi_p + \varphi_\alpha = 0$ and $\phi_p + 2\varphi_\alpha = \pm\pi$ the energy reduces to:

$$\langle H\rangle = \sum_p [\varepsilon_p(1-cos\theta_p) + \frac{1}{2}\Delta_p sin\theta_p + \alpha\gamma_p sin\theta_p]$$
$$+\Omega_0[\alpha^2 + \frac{1}{2}(cosh\Theta_0 - 1) + \frac{g_0}{2}(\alpha^2 + \frac{1}{2}sinh\Theta_0)^2] \quad (5.77)$$
$$+\sum_{p\neq 0}[\Omega_p[cosh\Theta_p - \frac{1}{2}] + \frac{g_0}{2}[\frac{1}{4}sinh^2\Theta_p + (\frac{\alpha^2}{2} + \frac{1}{4}\sinh\Theta_0)sinh\Theta_p]]$$

Since all the bosons would be in condensed state at $T = 0$ one can neglect the bosonic terms with $p \neq 0$.

Now if we introduce the parameters:

$$cos\theta_p = \frac{\varepsilon_p}{E_p} \quad (5.78)$$

$$sin\theta_p = \frac{-|\tilde{\Delta}_p|}{E_p} \quad (5.79)$$

$$cosh\Theta_p = \frac{\tilde{\varepsilon}_p}{E_p^b} \tag{5.80}$$

$$sinh\Theta_p = \frac{-2|g|}{E_p^b} \tag{5.81}$$

where $E_p = \sqrt{\varepsilon_p^2 + |\tilde{\Delta}_p^2|}$ and $E_p^b = \sqrt{\tilde{\varepsilon}_p^2 - 4|g|^2}$ with $\tilde{\Delta}_p = \Delta_p/2 + \alpha\gamma_p$, $\tilde{\varepsilon}_p = \Omega_p + 2g_0 N_0$ and $g = (g_0/2)(\alpha^2 + (1/2)sinh\Theta_0)$. With these parameters the energy eigenvalue can be written as:

$$\langle H \rangle = \sum_p \left[(1 - \frac{\varepsilon_p}{E_p})\varepsilon_p - \frac{\tilde{\Delta}_p^2}{E_p} + \Omega_0 N_0 + \frac{2g^2}{g_0} \right] \tag{5.82}$$

This energy eigenvalue converges to the known values for both BCS and BEC limits.

5.5 Variational Treatment (T=0)

Now that we have the Hamiltonian that describes the system, we will next evaluate the expectation value in our trial coherent state , and then optimize this Hamiltonian by using the variational method. Namely by varying the parameters θ, Θ, and α we will minimize the energy of the system.

Minimizing eq.5.77 with respect to θ_p :

$$\frac{\partial \langle H \rangle}{\partial \theta_p} = \sum_p [\varepsilon_p sin\theta_p + \frac{\Delta_p}{2} cos\theta_p + \gamma_p \alpha cos\theta_p] \tag{5.83}$$

$$0 = \varepsilon_p sin\theta_p + \left(\frac{\Delta_p}{2} + \gamma_p\alpha\right) cos\theta_p \tag{5.84}$$

$$tan\theta_p = -\frac{\Delta_p}{2\varepsilon_p} - \frac{\gamma_p}{\varepsilon_p}\alpha \tag{5.85}$$

At this point it is important to check the BCS limit. In our model this is where $\alpha = 0$ which then leads to the known gap equation and parameter;

$$tan\theta_p = -\frac{\Delta_p}{2\varepsilon_p} \tag{5.86}$$

This is a very similar expression for the gap parameter Δ to the one we have found for usual BCS system eq.5.23. The difference between these two gap parameters comes from the fact that the usual expression was calculated for mean field approximated Hamiltonian.

Using this expression one can rewrite the expectation value of the Hamiltonian as:

$$\begin{aligned}\langle H\rangle &= \sum_p \left(\varepsilon_p + \left(-\varepsilon_p^2 - (\alpha\gamma_p + \frac{\Delta_p}{2})^2\right)\frac{cos\theta_p}{\varepsilon_p}\right) \\ &+\Omega_0\left(\alpha^2 + \frac{1}{2}\left(cosh\Theta_0 - 1\right)\right) + \frac{g_0}{2}\left(\alpha^2 + \frac{1}{2}sinh\Theta_0\right)^2\end{aligned} \tag{5.87}$$

The minimization with respect to Θ_0 (as we have neglected $p \neq 0$ terms, Θ_0 is the only relevant term) is:

$$\frac{\partial\langle H\rangle}{\partial\Theta_0} = \frac{\Omega_0}{2}sinh\Theta_0 + g_0(\alpha^2 + \frac{1}{2}sinh\Theta_0)\frac{1}{2}cosh\Theta_0 = 0 \tag{5.88}$$

After a little algebra one can show that:

$$\alpha^2 + \frac{1}{2} sinh\Theta_0 = \frac{\alpha^2\Omega_0}{\Omega_0 + \frac{g_0}{2} cosh\Theta_0} \tag{5.89}$$

Using this condition one can further rewrite the Hamiltonian as :

$$\begin{gathered}\langle H\rangle = \sum_p \left(\varepsilon_p + \left(-\varepsilon_p^2 - (\alpha\gamma_p + \frac{\Delta_p}{2})^2\right) \frac{cos\theta_p}{\varepsilon_p}\right) \\ +\Omega_0 \left(\alpha^2 + \frac{1}{2}(cosh\Theta_0 - 1)\right) + \frac{g_0}{2}\left(\frac{\alpha^2\Omega_0}{\Omega_0 + \frac{g_0}{2} cosh\Theta_0}\right)^2\end{gathered} \tag{5.90}$$

The last minimization is with respect to parameter α:

$$\begin{gathered}\frac{\partial \langle H\rangle}{\partial\alpha} = \sum_p \left(-2\gamma_p \left(\alpha\gamma_p + \frac{\Delta_p}{2}\right) \frac{cos\theta_p}{\varepsilon_p}\right) \\ +2\Omega_0\alpha + g_0 \left(\frac{\alpha^2\Omega_0}{\Omega_0 + \frac{g_0}{2} cosh\Theta_0}\right)\left(\frac{2\alpha\Omega_0}{\Omega_0 + \frac{g_0}{2} cosh\Theta_0}\right) = 0\end{gathered} \tag{5.91}$$

which gives us the last condition:

$$\alpha^3 \left(\frac{2g_0}{(1 + \frac{g_0}{2\Omega_0} cosh\Theta_0)^2}\right) + \alpha\left(2\Omega_0 - \frac{2\gamma_p^2}{\varepsilon_p} cos\theta_p\right) - \left(\frac{\Delta_p\gamma_p}{\varepsilon_p}\right) cos\theta_p = 0 \tag{5.92}$$

By using this last condition the minimized Hamiltonian for an individual p can be written as:

$$\begin{aligned}\langle H\rangle_p = \varepsilon_p + \left(-\varepsilon_p^2 - \left(\alpha\gamma_p + \frac{\Delta_p}{2}\right)^2\right)\left(\frac{cos\theta_p}{\varepsilon_p}\right) + \left(\frac{\Omega_0}{2}\right)\left(\alpha^2 + cosh\Theta_0 - 1\right) \\ + \left(\frac{\Delta_p}{2} + \gamma_p\alpha\right)\left(\frac{\gamma_p\alpha}{2}\right)\left(\frac{cos\theta_p}{\varepsilon_p}\right)\end{aligned} \tag{5.93}$$

Writing the total number of particles in the system as $N = 2N_b + N_f$; whereN_b is the number of bosons and N_f is the number of fermions in the system. Assuming that $N_b \approx N_0$ since at $T = 0$ almost all molecules are in condensed state:

$$\begin{aligned} N = 2N_b + N_f = 2\left\langle c^\dagger c\right\rangle + \sum_p \left\langle a_p^\dagger a_p\right\rangle \\ N = \left\langle 4K_{30} - 1\right\rangle + \sum_p \left\langle 2J_{3p} + 1\right\rangle \\ N = \left(2\alpha^2 + cosh\Theta_0 - 1\right) + \sum_p (1 - cos\theta_p) \end{aligned} \tag{5.94}$$

Here one should notice that at the pure BCS limit there won't be any molecules and all the particles will be in Cooperpair states. Therefore one will have $\alpha = 0$ as well as $\Theta_0 = 0$ which can be called as BCS limit conditions. And for the pure BEC limit case one will have all the particles in a condensed molecule state, so $\alpha = 1$, and θ_p and Δ_p will be zero. At both limits γ_p should be zero since there will be no interaction between atoms and molecules. If we impose these conditions to see the limit values of the ground state energy:

$$\langle H\rangle_{BCS} = \varepsilon_p - \left(\varepsilon_p + \frac{\Delta_p^2}{4\varepsilon_p}\right) cos\theta_p \tag{5.95}$$

and the BEC limit gives:

$$\langle H\rangle_{BEC} = \frac{\Omega_0}{2} cosh\Theta_0 \tag{5.96}$$

The chemical potential of the system can be written as:

$$\frac{\partial E}{\partial N} = \frac{\partial E}{\partial \theta_p}\frac{\partial \theta_p}{\partial N} + \frac{\partial E}{\partial \alpha}\frac{\partial \alpha}{\partial N} + \frac{\partial E}{\partial \Theta_0}\frac{\partial \Theta_0}{\partial N} \tag{5.97}$$

Using eq.5.93 and eq.5.94, one can write:

$$\begin{aligned}\frac{\partial E}{\partial N} = &\left[-\left(\varepsilon_p^2 + \left(\alpha\gamma_p + \frac{\Delta_p}{2}\right)^2\right) + \left(\frac{\Delta_p}{2} + \gamma_p\alpha\right)\left(\frac{\gamma_p\alpha}{2}\right)\right]\left(\frac{-sin\theta_p}{\varepsilon_p}\right)\left(\frac{1}{sin\theta_p}\right)\\ &+\left(-2\gamma_p\left(\alpha\gamma_p + \frac{\Delta_p}{2}\right)\frac{cos\theta_p}{\varepsilon_p} + \Omega_0\alpha + \frac{\gamma_p^2\alpha}{2\varepsilon_p}cos\theta_p\right)\left(\frac{1}{4\alpha}\right)\\ &+\left(\frac{\Omega_0}{2}sinh\Theta_0\right)\left(\frac{1}{sinh\Theta_0}\right)\end{aligned} \tag{5.98}$$

$$\begin{aligned}\frac{\partial E}{\partial N} = \varepsilon_p + \frac{(\alpha\gamma_p + \frac{\Delta_p}{2})^2}{\varepsilon_p} - \left(\frac{\Delta_p}{2} + \gamma_p\alpha\right)\left(\frac{\gamma_p\alpha}{2\varepsilon_p}\right)\\ - \left(\gamma_p^2 + \frac{3}{4}\Delta_p\frac{\gamma_p}{\alpha}\right)\frac{cos\theta_p}{4\varepsilon_p} + \frac{3\Omega_0}{4}\end{aligned} \tag{5.99}$$

BCS limit of this chemical potential gives us:

$$\mu_{BCS} = \varepsilon_p + \frac{\Delta_p^2}{4\varepsilon_p} - \frac{3}{16}\frac{\Delta_p}{\varepsilon_p}cos\theta_p + \frac{3}{4}\Omega_0 \tag{5.100}$$

This chemical potential is positive as it is expected for a BCS system. And BEC limit gives us:

$$\mu_{BEC} = \frac{3}{4}\Omega_0 \tag{5.101}$$

which has a negative value as one would expect for a BEC system. Here one should note that $\Omega_0 = 2\nu - 2\mu$ and $\nu = \mu_B(B - B_0)$ where μ_B is the magnetic moment difference between open and closed channel, and at the BCS limit $B >> B_0$ and at the BEC limit $B << B_0$.

Chapter 6

Conclusions

Ultracold atomic gases have unique features which enable experimentalists to work on different aspects of the interacting fermions and bosons. Recent experiments showed that as the interaction between fermionic atoms (such as K,Li,Rb) increased through the help of Feshbach resonances, a continual change occurs from a BCS state of Cooper pairs to a BEC state of diatomic molecules. This phenomenon is called BCS-BEC Crossover. The standard BCS mean field theory of superconductivity was used to describe the whole crossover resulting a useful approximation, but as of today there is no exact analytical solution for this many-body problem.

In this thesis we have worked to find the best variational analytical solution to BCS-BEC Crossover problem at T=0. We obtained the ground state of the lowest energy from variation of the trial energy based on the generalized double-coherent trial wave function. It was shown that the coupled BCS-

BEC systems are in generalized SU(2)$\otimes$ SU(1,1) coherent states. Using this state as our trial wavefunction we calculated the energy eigenvalue and the chemical potential for the ground state and the limit values of the chemical potentials found to be consistent. We have developed the Hamiltonian to be the best fit to the problem among several other possibilities. This work can be extended to $T > 0$ case to find the thermodynamic parameters of the system. Further generalization of this work include addition of spin-orbit coupling terms to the Hamiltonian [61]. Furthermore, this new type of superfluid differs from ^{3}He, conventional and high-T$_c$ superconductors in its high critical temperature with respect to the Fermi temperature, $T_c/T_F \approx 0.2$ and this is the reason for these systems to be called *high-temperature superfluidity*. However, the crossover and high-T$_c$ problems share several features; while in the crossover regime the pair size is comparable to interparticle spacing, in high-T$_c$ superconductors the correlation length is comparable to the distance between electrons, therefore both systems are composed of strongly correlated fermions, and in both cases above the phase transition temperature correlations are still strong enough to form uncondensed pairs at finite momentum. Due to this resemblance between the two, theoretical work on crossover region helps us to understand the theory of high-T$_c$ superconductors. In fact, since the BCS-BEC crossover has been experimentally realized, ultra cold neutral alkali atoms gases have become a new lab not only in condensed matter physics and atomic physics but also in nuclear physics and hadron physics[42–44, 62].

Appendix A

Fano-Feshbach Resonances

Herman Feshbach was working on nuclear scattering when he realized that there can be resonant scatterings between a free nucleon and a nucleus. He showed that this can happen when the scattering energy(open channel) between the nucleon and nucleus is equal to the bound state energy(closed channel).

This phenomenon can be observed for the atomic systems too. Consider two atoms one of which has more than one hyperfine state approaching each other in an open channel. Since the z- component of magnetic moment is different for different channels the relative energy of the two atoms can be adjusted by tuning the applied magnetic field:

$$\Delta E = \Delta \mu \cdot B \tag{A.1}$$

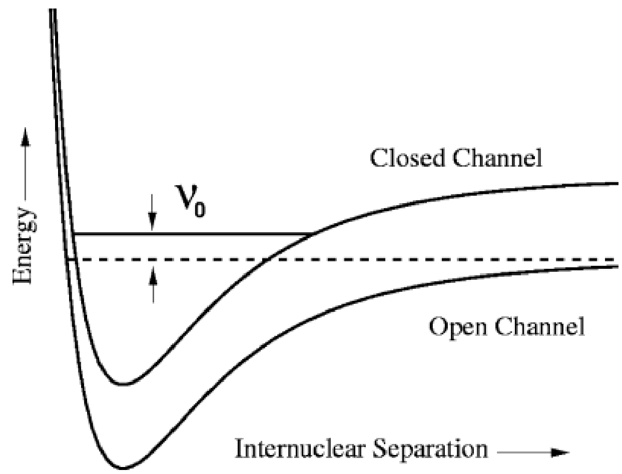

Figure A.1: Feshbach mechanism for nuclear scattering; the relative position of the closed channel(the bound state energy) with respect to open channel (scattering energy) can be changed by tuning the applied magnetic field.

It is possible to have $\Delta E = E_{closed} - E_{open} = |E_0|$ where E_0 is the binding energy of a particular bound state. In this case we can say that the bound state in the closed channel is degenerate with the scattering state in the open channel. In this limit that the detuning parameter $\delta = \Delta\mu \cdot B - |E_0|$ is almost zero the two channels would be strongly hybridized.

The interaction potential between alkali cold atoms depends on the internal structure of the two colliding atoms. Since the hyperfine interaction(V_{hf}) is not diagonal in the total electronic spin $S = s_1 + s_2$ of the two atoms there is a coupling between singlet and triplet potentials[63]:

$$V_{hf} = a_{hf}(\mathbf{s_1} \cdot \mathbf{i_1} + \mathbf{s_2} \cdot \mathbf{i_2}) = \frac{a_{hf}}{2}\mathbf{S} \cdot (\mathbf{i_1} + \mathbf{i_2}) + \frac{a_{hf}}{2}(\mathbf{s_1} - \mathbf{s_2}) \cdot (\mathbf{i_1} - \mathbf{i_2}) \quad (A.2)$$

where a_{hf} is the hyperfine constant and i_1, i_2 are the nuclear spins of the two atoms. The second term is the coupling between the symmetric (triplet) electronic spin states to antisymmetric (singlet) electronic spin states. The singlet potential is called “closed channel” since the singlet continuum states are not available as final scattering states because of the energy conservation. When the incoming state is resonant with the bound state in the singlet potential then the energy difference between the incoming state and the bound state can be changed by changing the applied magnetic field, which is called “Feshbach resonance”.

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