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THEORETICAL INVESTIGATION OF THE COEXISTENCE OF SUPERCONDUCTIVITY AND FERROMAGNETISM IN SUPERCONDUCTOR CeO 1x F x BiS 2

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THEORETICAL INVESTIGATION OF THE COEXISTENCE OF SUPER-CONDUCTIVITY AND FERROMAGNETISM IN SUPERCONDUCTOR $CeO_{1-x}F_xBiS_2$

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$\overline{Signature\ of\ Author}$

This Work is Dedicated To My Parents

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Bahir Dar Ethiopia

Amanu Andualem

Date: ....

Abstract

This research work deals with the theoretical investigation of the coexistence of superconductivity and ferromagnetism in superconductor $CeO_{1-x}F_xBiS_2$ ($x = 0 - 1.0$). By developing a model Hamiltonian for the system and using the Green's function formalism and equation of motion method, we have obtained expressions for superconducting transition temperature (T_c), magnetic order temperature (T_m), superconducting order parameter (Δ) and magnetic order parameter (η). By employing the experimental and theoretical values of the parameters in the obtained expressions, phase diagrams of energy gap parameter versus transition temperature (superconducting transition temperature versus magnetic order parameter and magnetic order temperature versus magnetic order parameter) are plotted separately. By combining the phase diagrams of superconducting transition temperature versus magnetic order parameter and magnetic order temperature versus magnetic order parameter, we have demonstrated the possible coexistence of superconductivity and ferromagnetism in $CeO_{1-x}F_xBiS_2$ superconductor. Our finding is in agreement with previous experimental findings.

Key words: Superconductivity, ferromagnetism, coexistence, $CeO_{1-x}F_xBiS_2$, Green's function.

CHAPTER 1

General Introduction

The phenomenon of superconductivity, in which the electrical resistance of certain materials vanish at low temperature, is one of the most interesting and sophisticated concept in condensed matter physics. It was first discovered by a Dutch Physicist Heike Kamerlingh Onnes in 1911 [1]. As shown in Fig.(1.1), by reducing the temperature of mercury(Hg) using liquid helium as a coolant, he observed that, the resistivity of Hg abruptly fell to zero at a critical temperature of about 4.2K. This observation was made possible by the liquefaction of helium in 1908 in the same laboratory [2]. Superconductivity is somewhat

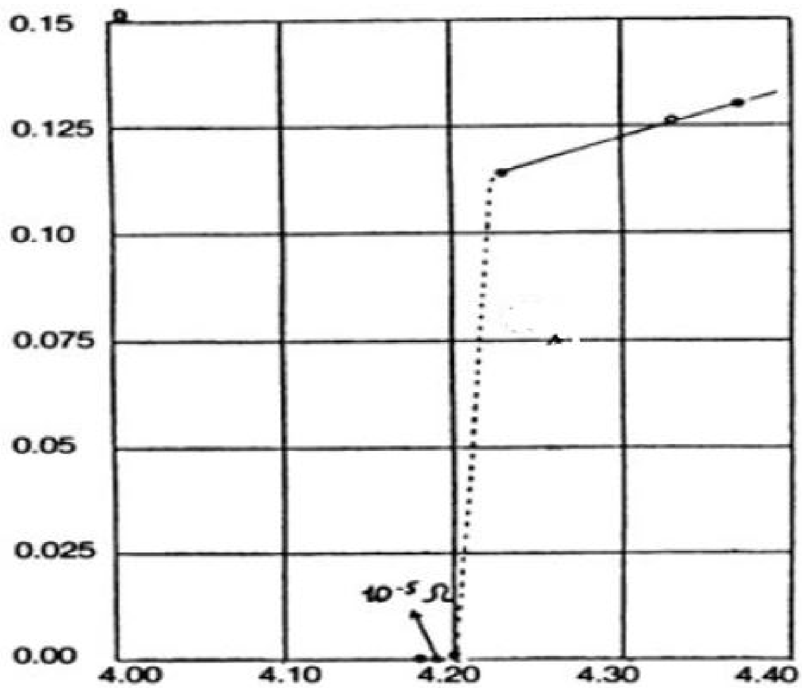

Figure 1.1: The resistivity of mercury as a function of temperature, produced in 1911 at the laboratory in Leiden [1].

related to the phenomena of superfluidity (in ^3He and ^4He) and Bose-Einstein condensation (in weakly interacting boson systems) [3]. Microscopically, superfluidity in ^3He is most closely related to superconductivity since both phenomena involve the condensation of fermions, whereas in ^4He it is the bosons that condense.

Superconductors have the ability to conduct electricity without loss of energy. When current flows in an ordinary conductor, some energy is lost. Atoms in these metal conductors form a vibrating lattice; the warmer the metal the more it vibrates. As the electrons move through the maze, they collide with tiny impurities in the lattice. When the electrons pump into these obstacles they fly off in all directions and lose energy in the form of heat. The movement of the superconducting paired electrons through the obstacles is quite different. As the superconducting paired electrons travel through the conductor they pass freely through the complex lattice. This is because the binding of electrons in pair eliminates the scattering process, which leads to zero resistivity and they can transmit electricity with no appreciable loss of current and energy.

The conditions in which a superconductor retains its superconducting properties is defined by its critical values [4]. These critical values are critical temperature T_c (the temperature at which the electrical resistance of the material drops to zero), the critical magnetic field H_c (the magnitude of the magnetic field, above which the superconductor loses its superconductivity) and the critical current density J_c (the current density above which the superconductor loses its superconductivity). They depend on the superconducting materials as illustrated in the Fig.(1.2) [5].

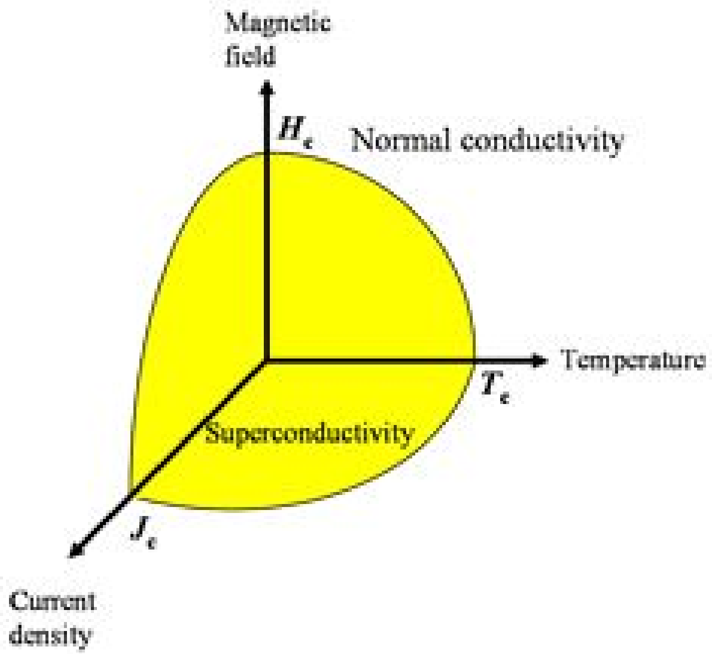

Figure 1.2: Graphical representation of the three parameters(T_c, H_c and J_c), to decide superconducting property.

Generally, High magnetic field, current density, and temperature are the three conditions that can break the superconductivity nature of a material.

Now, superconductivity is observed in quite a lot of elements, alloys, and inter-metallic compounds. Although metals are conductive, not all conducting metals are superconductive, and even some insulators are able to become superconductive under the right conditions.

Today, superconductivity is being applied to many diverse areas such as; theoretical and experimental science, military, transportation, power production, electronics, medicine, etc. [6].

1.1 Meissner Effect

In 1933, Walther Meissner discovered that, superconductors are more than a normal perfect conductors of electricity and they also have an interesting magnetic property of excluding a magnetic field [7]. When a superconductor is cooled below its transition temperature in a magnetic field, it completely expels the magnetic flux from its interior and bent around it as shown in Fig.(1.3) below. This is because under the influence of a magnetic field,

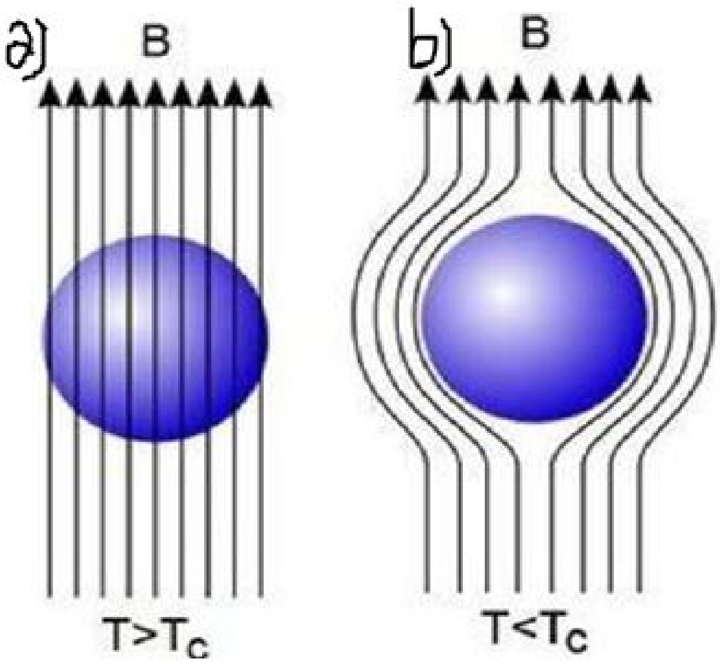

Figure 1.3: a) Above the transition temperature the magnetic field lines are penetrating the sphere, b) Below the transition temperature the magnetic field lines are ejected from the sphere.

surface currents that flow without resistance develop to create magnetization within the superconductor which is equal and opposite to the magnetic field, resulting in canceling out the magnetic field everywhere within the superconductor. This results the superconductor to have a magnetic susceptibility(χ_m) of -1, meaning it exhibits perfect diamagnetism. While many materials exhibit some small amount of diamagnetism, superconductors are strongly diamagnetic.

One of the most well known demonstrations of the Meissner effect is its ability to make a magnet levitate above a superconductor. When a magnet is placed above a superconductor, the repelling force can be stronger than gravity, allowing the magnet to levitate above the superconductor. This is not an entirely stable configuration, giving the magnet the freedom to spin above the superconductor while it tries to orient its magnetic poles. If the magnetic field is removed or the superconductor raises above the critical temperature, the surface currents and magnetization disappear, and the magnet will no longer levitate.

While the effects of flux pinning may appear similar to the levitating magnets caused by the Meissner effect, the cause behind flux pinning differs in some ways. For flux pinning to occur, the superconducting material either needs to be very thin or it needs to be a Type II superconductor. If it is thin or Type II superconductor, some of the magnetic field is allowed to pass through the superconductor, but only in specific spots, called flux tubes or a vortex. This passing of small amounts of the magnetic field through flux tubes at a small distance, to the order of (30-60)nm in metallic superconductors is called London penetration depth [5]. The reason that the magnetic field is allowed to pass through the superconductor at these flux tubes is, because there is no superconductivity within those regions. The superconductor tries to keep the flux tubes pinned to weaker parts of the superconductor, such as grain boundaries or other imperfections. When placed within a magnetic field, this pinning prevents the levitating magnet above a superconductor from moving easily without an applied force, keeping it steady in a stable location. This is also known as quantum locking.

1.2 Types of Superconductors

High magnetic fields destroy superconductivity and restore the normal conducting state. Depending on the characteristics of this transition there are two types of superconductors. These are type I and type II superconductors [5, 8].

1.2.1 Type I Superconductors

Type I (soft) superconductors withstand or resist only weak magnetic fields, that is why they are called soft. They are conventional superconductors which can be described by the Bardeen, Cooper and Schrieffer (BCS) theory. They are also called elemental superconductors (all pure samples of superconducting elements, except Nb, V and Tc exhibit type-I behavior) [9]. It has only one critical magnetic field (H_c), as shown in Fig.(1.4).

The behavior of type I superconductors, at a given temperature T and in a uniform external magnetic field H, can be described as follows: if H is smaller than a critical value (H_c), the superconductor completely expels the magnetic flux from its interior (complete Meissner effect); but as the external field is increased above the critical value (H_c), the specimen becomes in the normal state (incomplete Meissener effect).

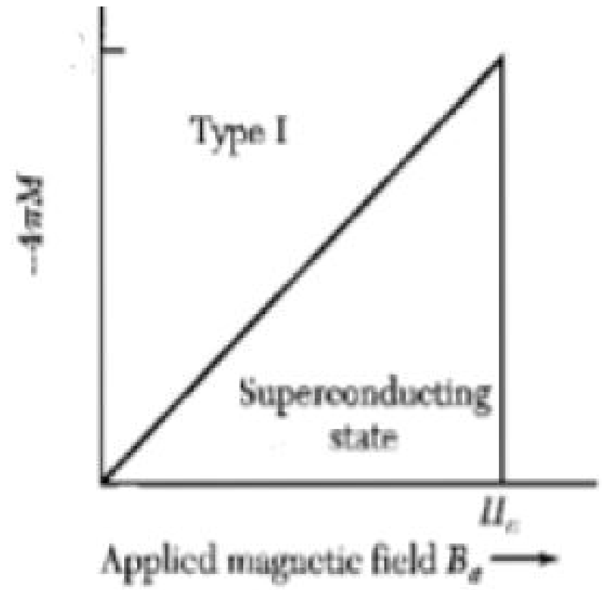

Figure 1.4: Magnetization versus applied magnetic field for Type I superconductors.

1.2.2 Type II Superconductors

Type II (hard) superconductors withstand relatively strong magnetic field as compared to type I superconductors. It has two critical magnetic fields which are lower critical magnetic field (H_{c1}) and upper critical magnetic field (H_{c2}) with a superconducting electrical properties up to a field denoted by H_{c2}. As shown in Fig.(1.5), if the magnetic field is lower than H_{c1} the specimen is in the superconducting state (complete Meissner effect). In the region between H_{c1} and H_{c2} ($H_{c1} < H_c < H_{c2}$) the flux density $B \neq 0$ and the Meissener effect is incomplete. In this region the state is intermediate as it contains partially both normal and the superconducting states, and is said to be in the vortex or mixed state.

A vortex is a magnetic flux quantum that penetrates the superconductor. Where the vortex appears the superconducting order parameter (Δ) drops to zero. Around the vortex a current starts to circulate. If the field is increased to the second critical field H_{c2} the specimen stops to be in the superconducting state. H_{c2} is usually bigger than H_c, that is why type II superconductors are typically used for building superconducting magnets.

Type II superconductors are attractive for technical applications due to their high current carrying capacity, such as generation of strong magnetic fields for particle accelerators, nuclear fusion reactors, magnetic resonance imaging (MRI), magnetic levitation (Maglev), and as well as measuring energy technology.

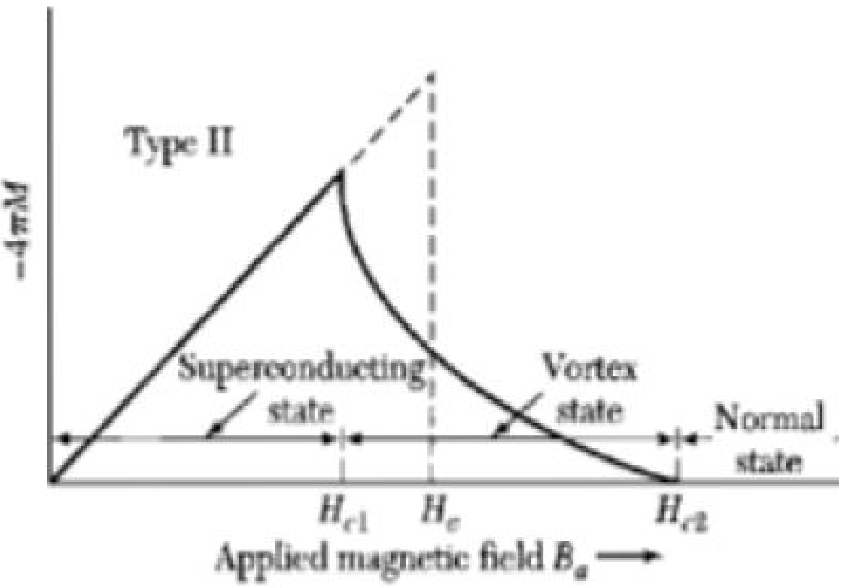

Figure 1.5: Magnetization versus applied magnetic field for Type II superconductors.

1.3 The BCS Theory of Superconductors

Early researchers suggested that fewer atomic vibrations would permit electrons to pass more easily. However, this predicts a slow decrease of resistivity with temperature. It soon became apparent that this simple idea could not explain superconductivity. In 1957, superconductivity was advanced by three American physicists, John Bardeen, Leon Cooper and John Schrieffer(BCS), which is nowadays, known as the BCS theory [10]. The basic principle of the BCS theory is that, electrons (fermions) pair up via phonon coupling and the pairs (bosons) condense into a single macroscopic quantum state and travel together cooperatively through the crystal lattice without scattering.

An attractive interaction between electrons can lead to a ground state separated from excited states by an energy gap. The critical field, the thermal properties, and most of the electromagnetic properties are consequences of the energy gap. The electron-lattice-electron interaction leads to an energy gap of the observed magnitude. The energy gap of superconductors is of entirely different origin and nature than the energy gap of insulators. In an insulator the energy gap is caused by the electron-lattice interaction. This interaction ties the electrons to the lattice. In a superconductor the important interaction is the electron-electron interaction which orders the electrons in **K**-space with respect to the Fermi gas of electrons. The transition in zero magnetic field from the superconducting state to the normal state is observed to be a second-order phase transition. At the second-order phase transition there is no latent heat, but there is a discontinuity in the heat capacity. Further, the energy gap decreases continuously to zero as the temperature is increased to the transition temperature T_c, as in Fig.(1.6). The minimum energy E_g required to break a Cooper pair inorder to create two quasi particle excitations is given by $E_g = 2\Delta(T)$ (where

$\Delta(T)$ is superconducting gap parameter).

$$2\Delta = 3.53 k_B T_c \tag{1.1}$$

The key consequences of the BCS theory include a connection of the superconducting gap parameter (Δ) to the transition temperature T_c and the Debby temperature ($\Theta_D = \frac{\hbar w_D}{k_B}$),

$$T_c = 1.14\Theta_D \exp(\frac{-1}{N(0)V}) = 1.14\Theta_D \exp(\frac{-1}{\lambda}) \tag{1.2}$$

where, N(0) is the density of states at the Fermi level, V is the attractive electron phonon interaction potential, $\lambda = N(0)V$, and is a coupling constant.
The gap parameter (Δ) at any temperature between the absolute zero and T_c is given by,

$$\Delta(T) = 3.06 k_B T_c (1 - \frac{T}{T_c})^{1/2} \tag{1.3}$$

This is the fundamental expression for a superconducting state and is a universal value for metals in the BCS approximation.

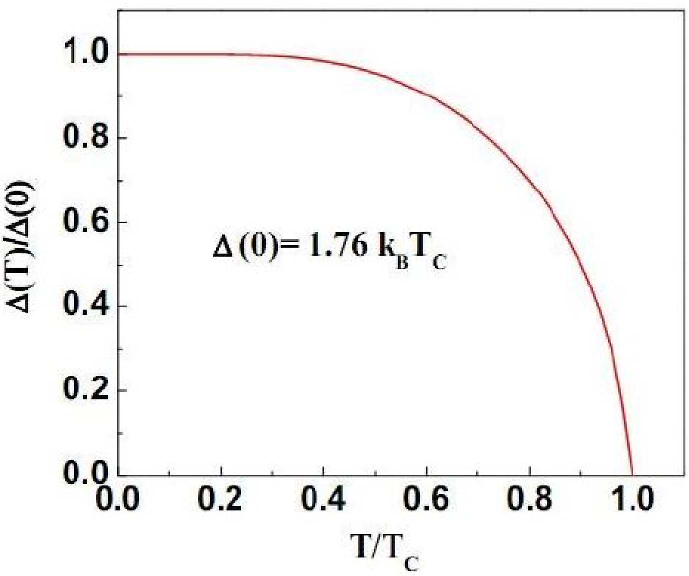

Figure 1.6: Variation of the reduced gap $\frac{\Delta(T)}{\Delta(0)}$ with the reduced temperature $\frac{T}{T_c}$ according to the BCS theory.

For weak coupling superconductors, the reduced gap $\frac{\Delta(T)}{\Delta(0)}$ is a universal function of the reduced temperature $\frac{T}{T_c}$, near the critical temperature T_c, so that the energy gap approaches zero continuously as T $\longrightarrow T_c$

$$\frac{\Delta(T)}{\Delta(0)} = 1.76(1 - \frac{T}{T_c})^{1/2} \tag{1.4}$$

In general, the main facts which the theory of superconductivity must explain are, a second order phase transition at the critical temperature T_c (in this case there is no change in entropy and latent heat at the critical temperature T_c), the Meissner effect (B=0), effects associated with infinite conductivity (R=0), and the dependence of T_c on isotopic mass $T_c\sqrt{M} = constant$ (which indicates that electron phonon interactions are primarily responsible for superconductivity).

1.3.1 Cooper Pairs

Leon Cooper (1956), showed that electrons which normally repel each other must feel an over whelming attractions in superconductors [10]. The pairing of electrons takes place through an intermediary of lattice vibrations known as phonon(bosons). According to the BCS theory, as an electron passes by a positive charged ion in the lattice of a superconductor, the electron polarizes or distorts the atom around it. This polarization of the lattice causes phonon to be emitted which form a trough of positive charges around the electron. Before the first electron passes by and the lattice springs back to its original position a second electron enters into the trough, and interacts into the polarization forming a Cooper pair. Therefore, it is this lattice vibration which causes the two electrons(which normally repel to each other) attract to each other to form Cooper pairs. That is, the forces exerted by the phonon overcome the natural repulsion of the electrons and are screened by phonon.

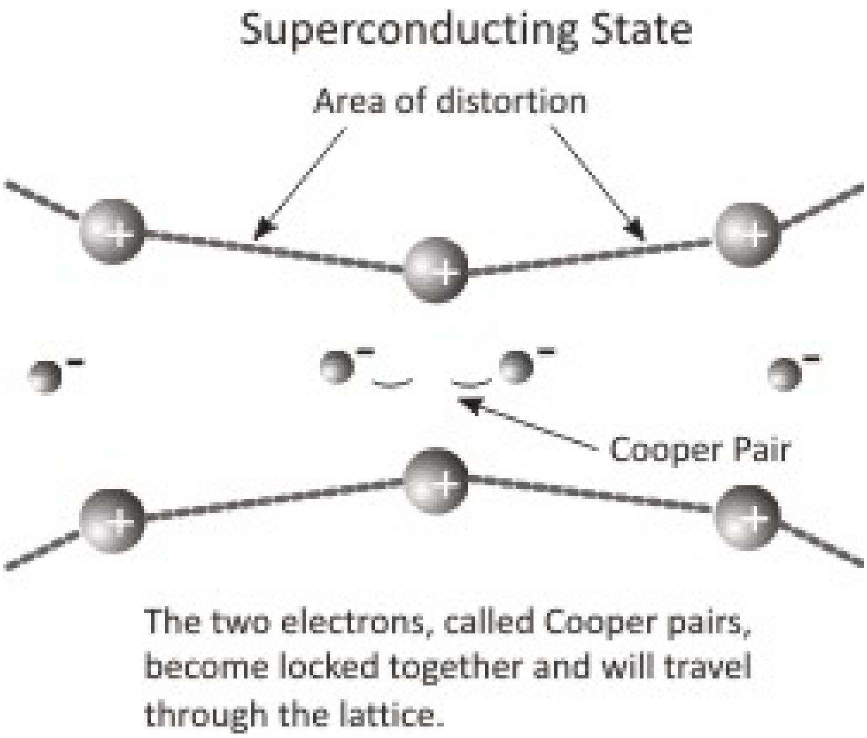

Figure 1.7: Schematic illustration of the formation of Cooper pairs.

1.4 Development of superconductivity

After Onnes discovered the superconductivity of mercury, conventional or low temperature superconductivity was observed in quite a lot of elements [3]. Many alloys and intermetallic compounds were also found to show conventional superconductivity. Of these, Nb_3Ge had the highest known T_c of 23.2K for long time. Due to this reason superconductivity seemed to be more or less closed subject until 1986 and thus did not promise widespread technological applications. It was well understood based on the BCS theory and extensions thereof that dealt with strong interactions. But in 1986 Bednorz and Muller discovered superconductivity in a lanthanum-based ($La_{2-x}Ba_xCuO_4$) perovskite material, which had a transition temperature of about 35K [3], with the layered perovskite cuprate La_2CuO_4. This discovery opened the gate widely and high T_c or unconventional superconductors continued to be discovered by using liquid nitrogen ($T_c = 77K$) as a coolant [11]. In high temperature superconductors magnetic fluctuations are believed to play the role of mediating for electrons pairing.

In the recent years, breakthrough discoveries have focused on layered superconducting materials. The discovery of new layered superconductors is one of the most important issues for the realization of T_c approaching to room temperature. The most outstanding example is Cu-oxide superconductors with the maximum critical temperature (T_c) of 164K for $HgBa_2Ca_2Cu_3O_{8+\delta}$ under high pressure [11]. In 2001, high-T_c superconductor ($T_c = 39K$) was discovered in the binary compound MgB_2 [11]. Due to the simple binary composition and low cost of the materials, it is one of the promising materials for applications on superconductivity. In 2008 another discovery of a high-T_c superconductor is accomplished in the layered materials with Fe-square lattice (conductive layers) with highest record of $T_c = 58K$ observed in $SmFeAsO_{1-x}F_x$ [12].

In 2012, novel layered superconductors which have a crystal structure similar to those of the Cu-oxide and Fe-based superconductors were discovered by Mizuguchi et al.[11, 13]. It has the characteristic structure of an alternate stacking of superconducting BiS_2 layers and blocking layers. In the conduction plane, the Bi and S atoms are alternately aligned and form a Bi-S square plane. The new superconducting family is called BiS_2-based superconductors. There are three types of BiS_2-based superconductors, $Bi_4O_4S_3$, $ReOBiS_2$ (Re=La, Ce, Pr, Nd, Yb, Sm), and $AeFBiS_2$ (Ae=Sr and Eu) with the highest record of T_c is 11K in $LaO_{0.5}F_{0.5}BiS_2$ [14]. The first member of the BiS_2-based superconducting family is $Bi_4O_4S_3$ and the second is $LaO_{1-x}F_xBiS_2$ [11]. At present, the studies of BiS_2-based superconductors have focused on the $ReO_{1-x}F_xBiS_2$ type because high quality samples of single and poly-crystals can be prepared. Furthermore, the physical properties, such as superconductivity and magnetism, dramatically change when changing the rare earth elements (Re) of the blocking layer. $CeO_{1-x}F_xBiS_2$ superconductor is one of $ReO_{1-x}F_xBiS_2$ layered compounds, with T_c can be increased from 3K for as grown (AG) sample to 8K by high pressure (HP) annealing at x = 0.7, with the ferromagnetic ordering temperature following the increase from 4.5K to 7.5K [15].

In this research work, we investigated theoretically the coexistence of superconductivity and ferromagnetism in $CeO_{1-x}F_xBiS_2$ compound.

CHAPTER 2

Literature Review

2.1 Introduction

In this chapter, we have presented a brief review of superconductivity and ferromagnetism. The crystal structure and the coexistence of superconductivity and ferromagnetism with regard to $CeO_{1-x}F_xBiS_2$ superconductor are also reviewed.

2.2 Superconductivity and Ferromagnetism

Ferromagnetism is a phenomenon by which a material can exhibit parallel alignment of moments resulting in a large net magnetization, even in the absence of a magnetic field [16]. It has a long-range magnetic ordering at the atomic level which causes unpaired electrons spin to line up parallel with each other in a microscopic region called domain. Within the domain, the magnetic field is intense but in the bulk sample the material will usually be unmagnetized because many domains will themselves be randomly oriented with respect to each other. The application of an external magnetic field results in an expansion of the domain with moments align with the field at the expense of those with anti-aligned moment.

In general, any current loop has a magnetic field and a corresponding magnetic moment. Similarly, the magnetic moments in a magnetized substance are associated with internal currents on the atomic level. Such currents arise from electrons orbiting around the nucleus. The total magnetic moment of an atom has orbital and spin contributions. For atoms or ions containing many electrons, the electrons in closed shells pair up with their spins and orbital angular momenta opposite to each other, a situation that results in a net magnetic moment of zero. However, atoms with an odd number of electrons must have at least one unpaired electron and a spin magnetic moment of at least one Bohr magneton. An unpaired outer electron can contribute both an orbital moment and a spin moment. For example, if the unpaired electron is in an s state, $L = 0$, and consequently the orbital moment is zero. However, if the unpaired electron is in a p or d state, $L \neq 0$, and the electron contributes both an orbital moment and a spin moment.

Furthermore, some compounds show superconductivity which coexist with long range magnetic ordering [18]. Since long range magnetic ordering usually competes with superconductivity, the materials possessing the coexistence of superconductivity and magnetism is a great interest for basic physics and applications. Superconductivity is associated with the pairing of electron states related to time reversal, while in the magnetic states the time-reversal symmetry is lost and therefore there is a strong competition with superconductivity [19]. Indeed, in conventional superconductors, local magnetic moments break up the spin-singlet Cooper pairs and hence strongly suppress superconductivity, an effect known as "pair-breaking". Therefore, a level of magnetic impurity of only one percent, can result in a complete loss of superconductivity. In a limited class of inter-metallic systems, superconductivity occurs even though magnetic ions with a local moment occupy all of one specific crystallographic site, which is well isolated and de-coupled from the conduction path.

2.3 Mechanism of Coexistence of Superconductivity and Ferromagnetism

The coexistence of superconductivity and ferromagnetism has been studied theoretically by Ginsburg [20] in 1957 and experimentally by Matthias et al. [21]. In fact $ErRh_4B_4$ was the first ferromagnetic superconductor in which superconductivity was found to exist in a small temperature interval with modulated ferromagnetic phase [22]. Furthermore, ferromagnetic superconductor has been experimentally established in URhGe [23], $ZrZn_2$ [24], UGe [25], and UIr [26].

Conventional BCS superconductors are characterized by a standard s-wave, spin-singlet pairing state with S=0, L=0 Cooper pairs. The two electrons of a pair have equal and opposite momenta $\vec{k_{i\uparrow}}$ and $-\vec{k_{i\downarrow}}$, and the wave function describing the pair consists of all states "i" occupied by the pair during its lifetime. In contrast to the standard s-wave pairing, the widely accepted mechanism of the Cooper-pairing in superfluid ^3He is based on an attractive interaction between the fermion (^3He) atoms due to a virtual exchange of spin fluctuations [27]. The coexistence of superconductivity and ferromagnetism in U-based compounds can be understood in terms of spin fluctuation model. In the ternary compounds the ferromagnetism comes from the localized 4f electrons whereas the s-wave Cooper-pairs are formed by conduction electrons. In the vicinity of a ferromagnetic quantum critical point, critical magnetic fluctuations can mediate superconductivity by pairing the electrons in spin-triplet Cooper-pairs that is the equal spin pairing (ESP) states, $|\uparrow\uparrow>$ $(L = 1, S_z = 1)$ and $|\downarrow\downarrow>$ $(L = 1, S_z = -1)$, and the state $\frac{|\uparrow\downarrow>+|\downarrow\uparrow>}{\sqrt{2}}$ with orbital moment $L = 1$ and projection of spin momentum $S_z = 0$ [28].

Now, among various BiS_2-based compounds, characterized by different spacer layers, $CeO_{1-x}F_xBiS_2$ [15] with the coexistence of superconductivity and ferromagnetism at low temperature is of particular interest due to possibly the role of Ce 4f states in the electronic properties.

2.4 Crystal Structure of Superconductor $CeO_{1-x}F_xBiS_2$

The knowledge of interactions between different layers and their effect on the electronic transport mechanisms is one of the important scientific fields in layered multi-band systems. The discovery of superconductivity in BiS_2-based materials has stimulated large interest aiming at the search of superconductors with higher transition temperature in this new family of layered chalcogenides. There are now several known BiS_2-based materials with majority of them having a general formula of $ReOBiS_2$ (Re=rare earth) with electronically active BiS_2-layers separated by ReO spacer layers [29]. Among those $CeO_{1-x}F_xBiS_2$ is one of the newly discovered superconductors with the crystal structure of tetragonal ($a = b \neq c, \alpha = \beta = \gamma = 90^o$) space group of P4/nmm or I4/mmm is basically composed of an alternate stacking of $CeO_{1-x}F_x$ and the BiS_2 layers [29, 30].

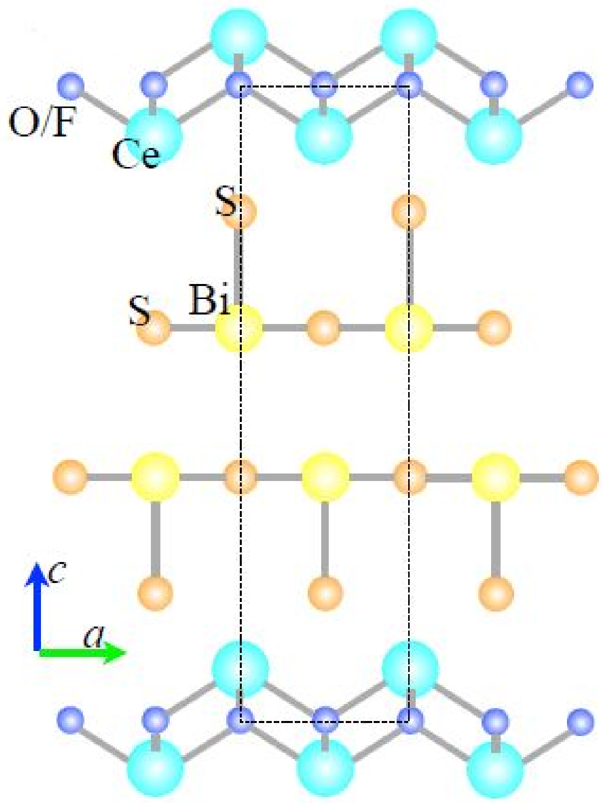

Figure 2.1: The crystal structure of superconductor $CeO_{1-x}F_xBiS_2$ [30].

The parent system ($CeOBiS_2$), without any fluorine doping is a metallic phase embedded in the morphological defects and at the sample edges of $CeOBiS_2$, while the bulk of the sample is semiconducting. Xing et al. firstly synthesized the $CeO_{1-x}F_xBiS_2$ polycrystalline samples [31]. The local structure of both BiS_2 active layer and $CeO_{1-x}F_x$ spacer layer change systematically as a function of F-substitution [15].

The enlarged XRD figure near the (110), (114) and (200) peaks for the as grown(AG) samples are shown in Fig.(2.2) [18]. Each of these present themselves as a single peak between $x = 0.0$ and 0.6. However, other peaks appear above $x = 0.7$ and become stronger with increasing F concentration. Furthermore, the peaks of the tetragonal phase seem to shift with increasing F concentration. These facts imply that another phase appears or the tetragonal structure is changed to monoclinic above $x = 0.7$. The observed peaks of $CeO_{1-x}F_xBiS_2$ samples may partly begin to be strained into a lower-symmetry phase due to lattice contraction upon F substitution.

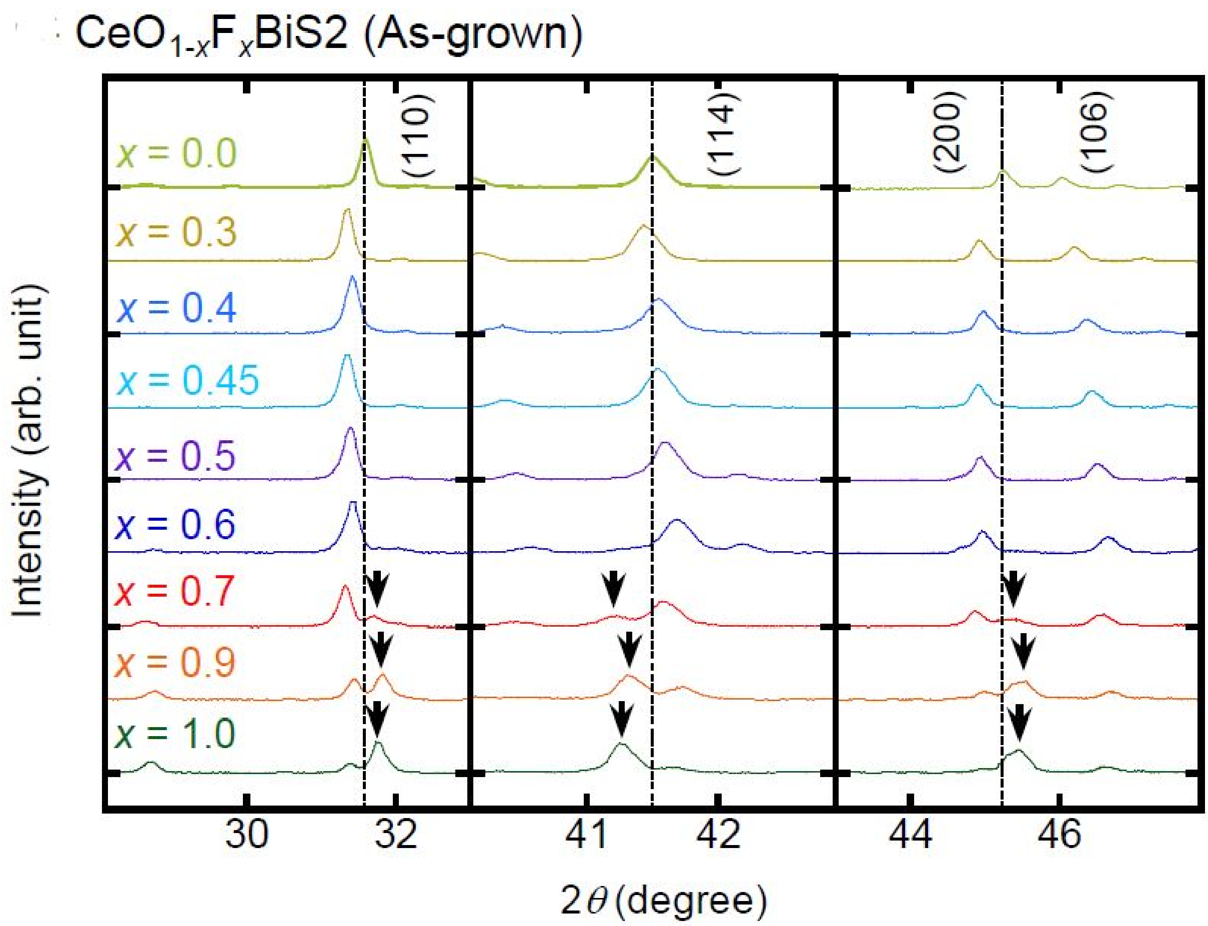

Figure 2.2: The powder X-ray diffraction profile for samples of superconductor $CeO_{1-x}F_xBiS_2$ ($x = 0.0 - 1.0$) [18].

As can be seen from Fig.(2.3) for the as-grown samples, the "a" lattice constant increases with increasing F concentration between $x = 0.0$ and 0.6, while it slightly decreases above $x = 0.7$. The lattice constant estimated from the peak positions is $4.0477\AA$ with F content [32], and almost the same for high pressure annealing.

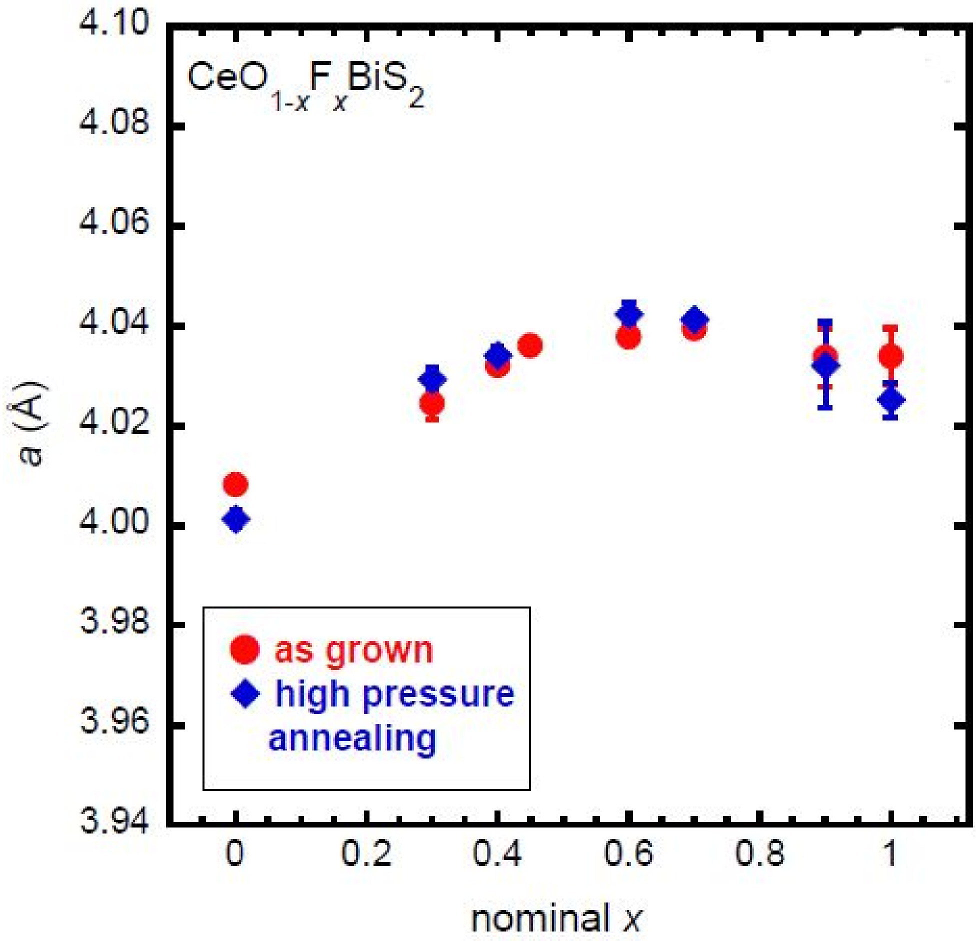

Figure 2.3: The variation of the lattice constants a with nominal x for as grown (AG) and high pressure(HP) samples of $CeO_{1-x}F_xBiS_2$ [18].

It can be observed from Fig.(2.4) that, the "c" lattice constant markedly decreases between x = 0.0 and 0.6 and keeps an almost constant value from x = 0.7 to 1.0. The c lattice constants as estimated from the peak positions is $c = 13.429\mathring{A}$ with F content for both as grown and HP samples [32].

This decrease in the c lattice constant between x = 0.0 and 0.6 indicates that F substitutes O as expected. After high pressure annealing, both a and c lattice constants exhibit almost the same behavior as the AG samples for all F concentrations. Therefore, the change of the crystal structure before and after high-pressure annealing is not large, but some local structures should be tuned, because superconducting properties significantly change after high-pressure annealing.

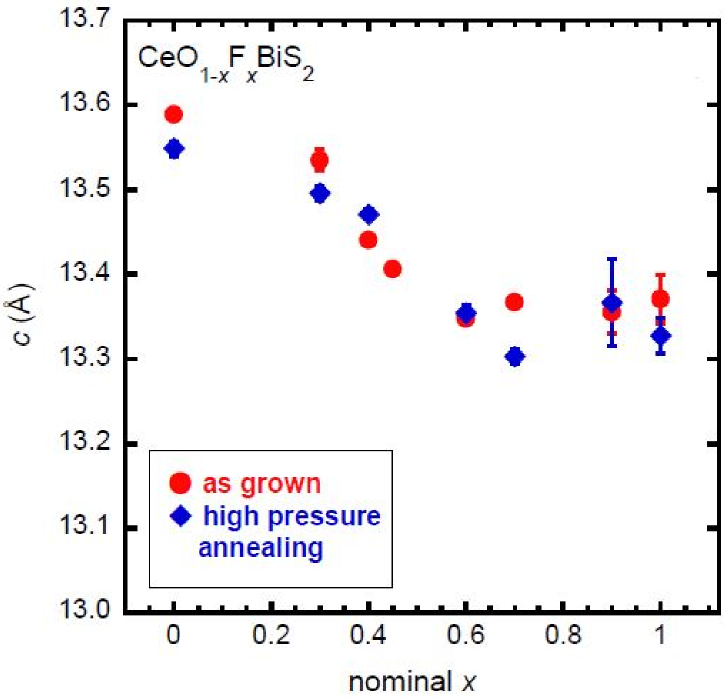

Figure 2.4: The variation of the lattice constants c with nominal x for AG and HP samples of $CeO_{1-x}F_xBiS_2$ [18].

The local crystal structure of $CeO_{1-x}F_xBiS_2$ has been determined by extended x-ray absorption fine structure (EXAFS) measurements as a function of F-content, providing atomic site selective information [15].

Ce L_3-edge EXAFS is used to study local structure of the $CeO_{1-x}F_x$ layer and Bi L_3-edge EXAFS is used to quantify local atomic displacements in the BiS_2 layer. The EXAFS measurements (on samples synthesized differently i.e. AG and HP annealed) reveal a systematic change in the local structure of the $CeO_{1-x}F_x$ and BiS_2-layers. The results show that the in-plane Bi-S ($Bi - S_1$) distance gets shorter (maximum change in the distance, $\Delta R_{max} \sim 0.08\mathring{A}$) with an elongation of the out-of plane Bi-S ($Bi - S_2$) distance ($\Delta R_{max} \sim 0.12\mathring{A}$) with increasing F-content [15]. The local atomic displacements in the $CeO_{1-x}F_x$ layer are much larger, with an elongation of Ce-O distance ($\Delta R_{max} \sim 0.2\mathring{A}$) and a contraction of $Ce - S_2$ distance ($\Delta R_{max} \sim 0.15\mathring{A}$). It is found that the HP annealing, that is known to improve superconducting properties, affects mainly the BiS_2 layer, with larger in-plane $Bi - S_1$ disorder. The results suggest that the BiS_2 and the $CeO_{1-x}F_x$ layers are decoupled at higher F-content due to increased $Bi - S_2$ distance.

Thus, coupling/decoupling of layers is the reason for the coexisting of superconductivity and ferromagnetism in this system.

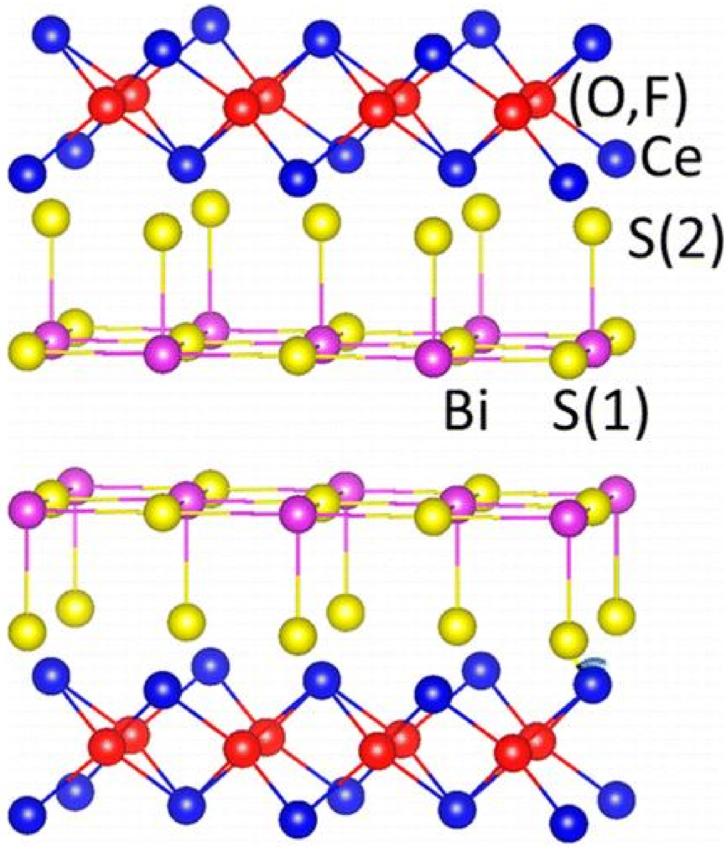

Figure 2.5: Local crystal structure representation of Ce(O,F) blocking layers and BiS_2 superconducting layers [15].

2.5 Electronic Properties of Superconductor $CeO_{1-x}F_xBiS_2$

The temperature dependence of resistivity for AG samples of $CeO_{1-x}F_xBiS_2$ (x=0-1.0) is shown in Fig.(2.6). The resistivity for all F doped samples increases with decreasing temperature. This implies that, for higher temperatures or in the normal-state region $CeO_{1-x}F_xBiS_2$ system has a semiconducting like behavior.

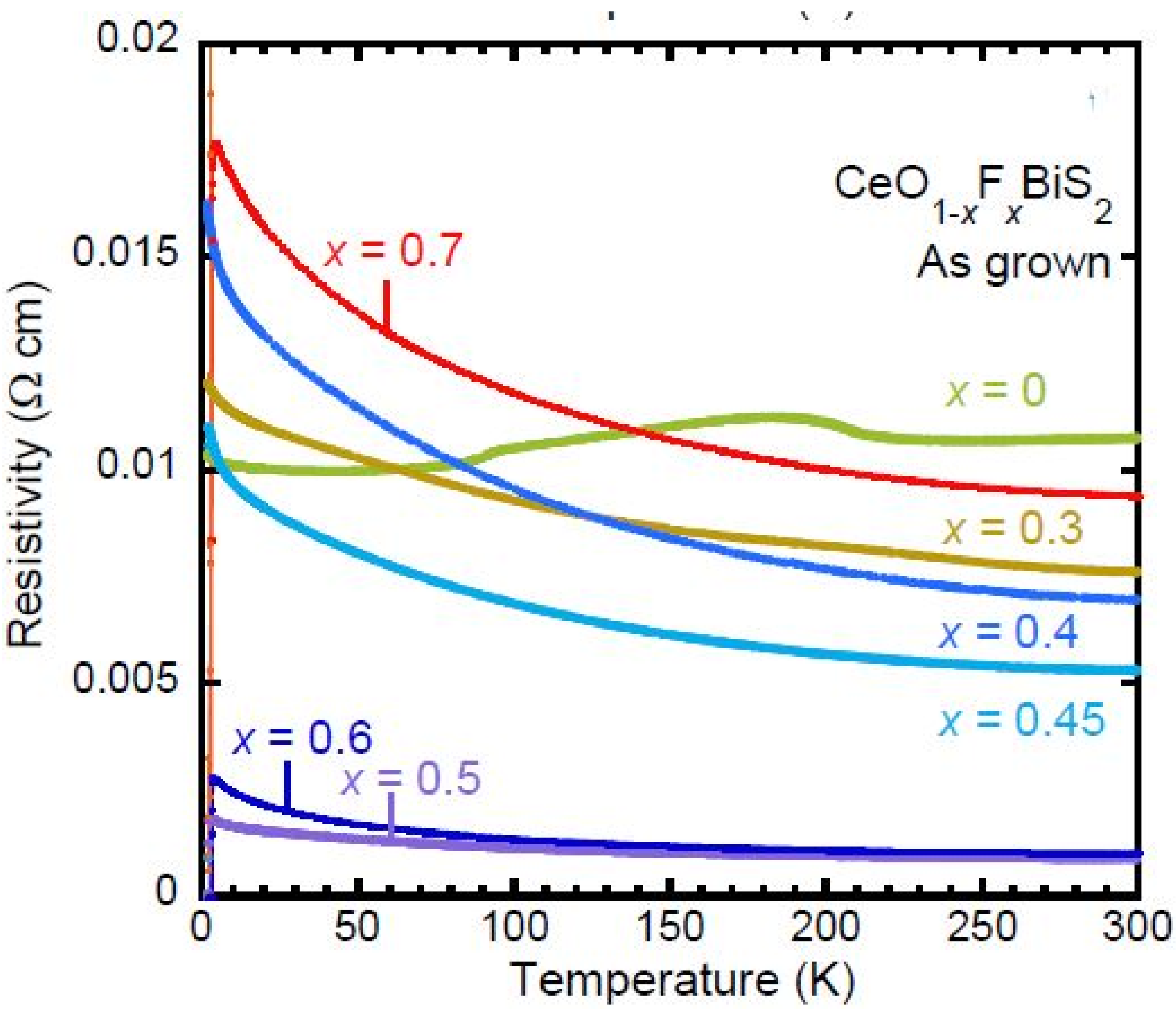

Figure 2.6: The temperature dependence of resistivity for AG samples of $CeO_{1-x}F_xBiS_2$ for large temperatures [18].

The low temperature region is enlarged in Fig.(2.7). The T_c^{onset} is regarded as the crossing point of the fitting lines for resistivity in the normal state near the transition and the drop area during the transition. The T_c^{zero} is estimated as the crossing point of the line for zero resistivity. Superconductivity does not appear between $x = 0.0$ and 0.4. Above $x = 0.45$, the onset of the superconducting transition is observed for all the samples. Zero resistivity is observed between $x = 0.45$ and 0.7 [18].

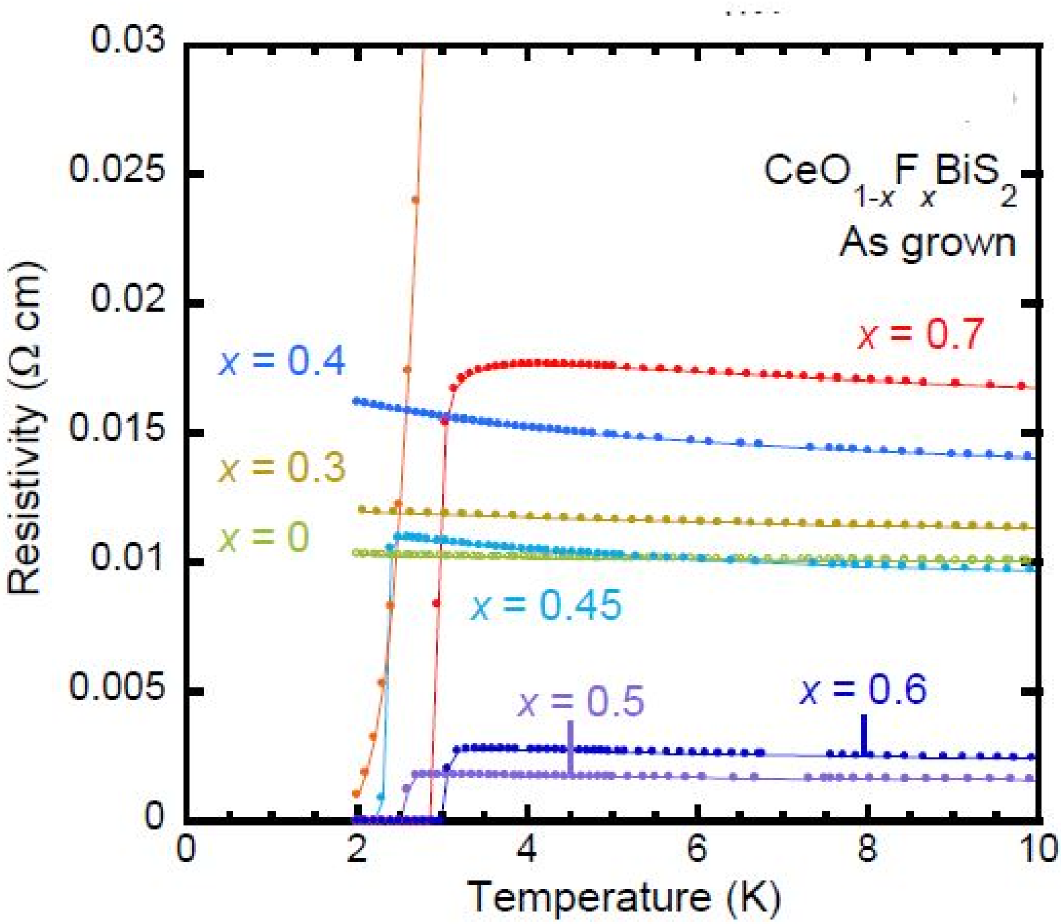

Figure 2.7: Temperature dependences of electrical resistivity for as grown $CeO_{1-x}F_xBiS_2$ enlarged at low temperature [11].

The temperature dependence of resistivity for $CeO_{1-x}F_xBiS_2$ $(x = 0 - 1.0)$ after high-pressure annealing is shown in Fig.(2.8) [18]. All the samples show a semiconducting behavior in the normal state. The samples above $x = 0.3$ exhibits the onset of the superconducting transition. A T_c^{onset} is observed around 3K for samples where x = 0.3, 0.4, 0.45, and 1.0. The sample with x = 0.6 shows the onset of superconducting transition around 6K. For x = 0.7 and 0.9, T_c^{onset} is observed around 8K. T_c^{zero} is not observed for $x < 0.6$ in the temperature range down to 2K. For $0.6 \leq x \leq 0.9$, bulk superconductivity is observed. Among them, $CeO_{0.3}F_{0.7}BiS_2$ shows the maximum T_c^{onset} of 8K. The fact that bulk superconductivity with higher T_c appears for $x \geq 0.6$ seems to be consistent with the observation of structural change revealed in Fig.(2.2).

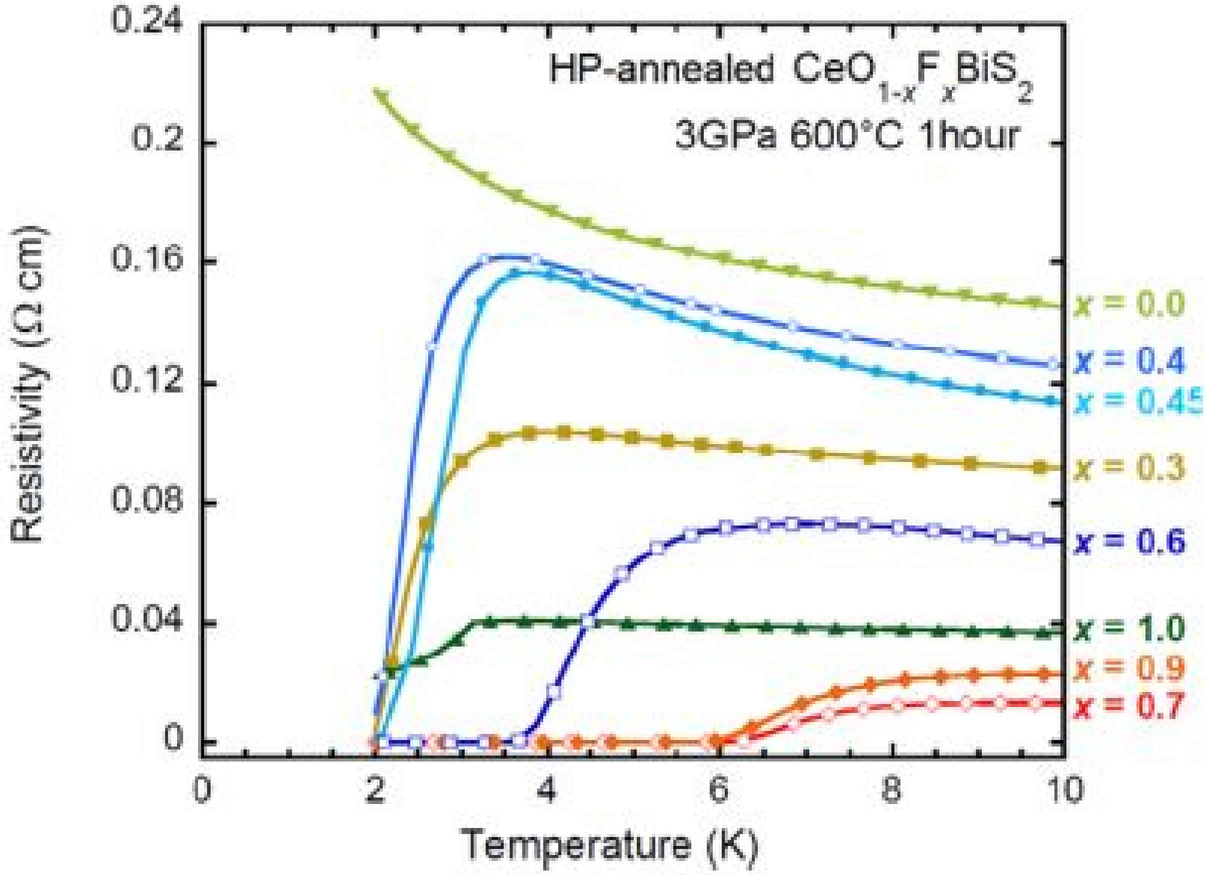

Figure 2.8: Temperature dependences of electrical resistivity for HP-annealed superconductor $CeO_{1-x}F_xBiS_2$. [11]

The temperature dependence of magnetic susceptibility for the AG samples of the superconductor $CeO_{1-x}F_xBiS_2$ is shown in Fig.(2.9) [18]. Paramagnetic behavior is observed for samples where x = 0.0 - 0.4. A superconducting transition appears around 2.5K for samples where x = 0.45, 0.5 and 0.6. In these samples, the magnetic susceptibility increases around 4.5K with decreasing temperature. Furthermore, x = 0.6 sample exhibits two anomalies at 4.5K and 7.5K. Above x = 0.7, the magnetic susceptibility largely increases at 7.5K. The increase of magnetic susceptibility suggests that two ferromagnetic phases with respect to magnetic transition temperatures of 4.5K and 7.5K exist.

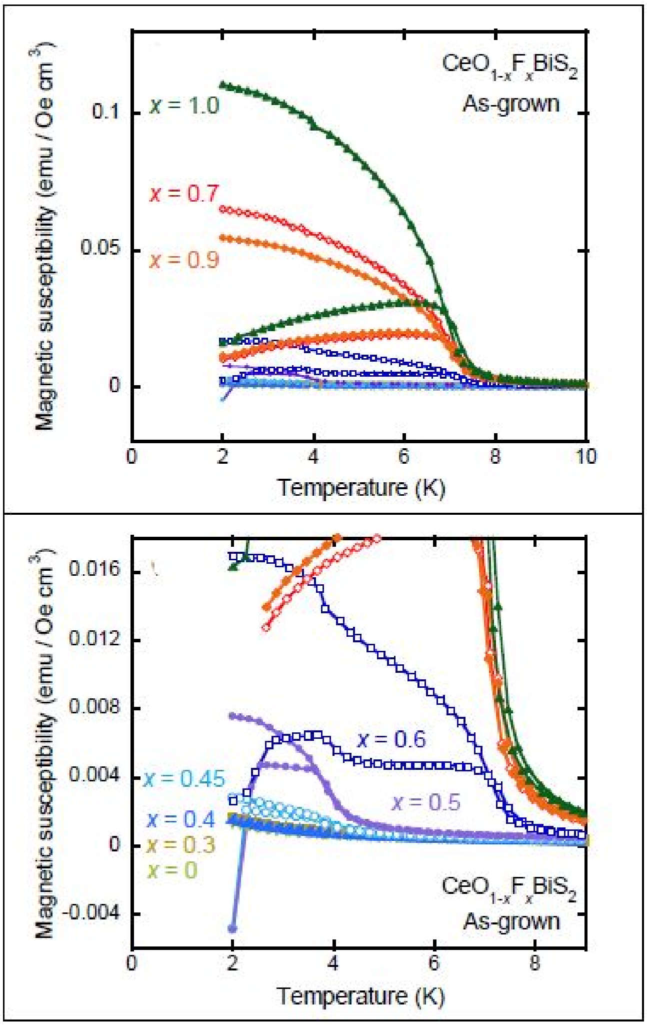

Figure 2.9: Variation of magnetic susceptibility with temperature for AG samples of $CeO_{1-x}F_xBiS_2$ [18].

Magnetic susceptibility measurements for HP samples are presented in Fig.(2.10) [18]. After high pressure annealing, superconductivity around 6K appears when x = 0.7 and 0.9. In this region, ferromagnetism at 7.5K is dominant. $CeO_{0.3}F_{0.7}BiS_2$ shows the strongest diamagnetic signal among all the samples, while exhibiting ferromagnetic ordering below 7.5K.

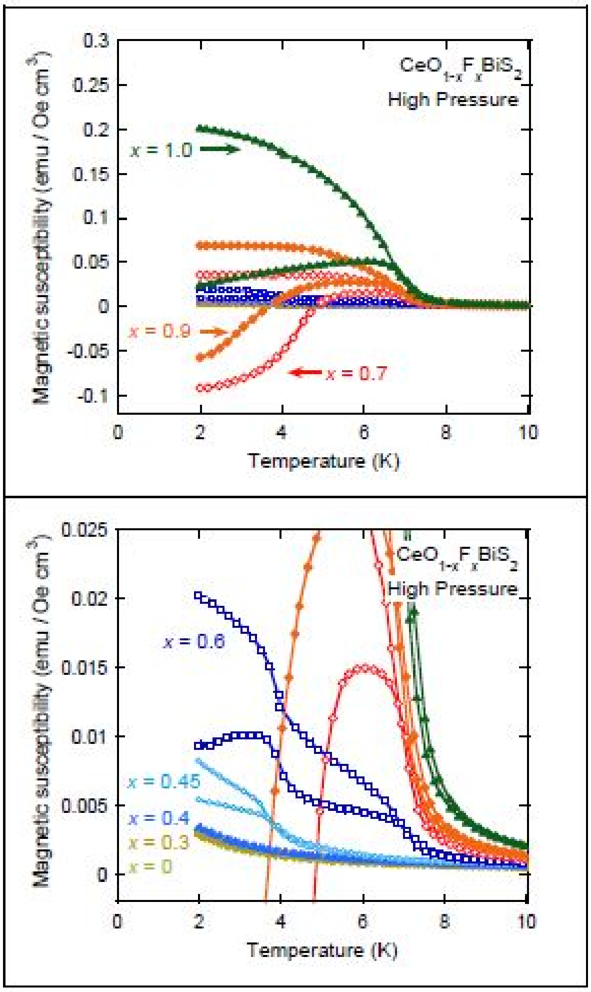

Figure 2.10: The temperature dependence of the magnetic susceptibility for HP samples of $CeO_{1-x}F_xBiS_2$ [18].

2.6 Coexistence of Superconductivity and Ferromagnetism in Superconductor $CeO_{1-x}F_xBiS_2$

The coexistence of superconductivity and ferromagnetism in $CeO_{1-x}F_xBiS_2$ system is due to a crossover of Ce 4f orbitals from itinerant to localized character driven by atomic correlations between the BiS_2 layers and the $CeO_{1-x}F_x$ spacer layers through $Ce - S_2 - Bi$ interaction channel [15]. The latter layer has no metallic d band and it is a narrow-gap semiconductor [14]. F substitution for O introduces charge carriers which contributes to both the superconducting BiS_2 and blocking CeO layers and change in the valence of Ce ion may have important role in the physical properties of $CeO_{1-x}F_xBiS_2$.

The electrical resistivity measurements revealed that superconducting transitions are observed for $x \geq 0.3$ in $CeO_{1-x}F_xBiS_2$, and T_c reaches 3K [11]. However, large diamagnetic signals were not observed in the magnetization measurements, indicating that the observed superconducting states were not bulk in nature in the as grown samples of $CeO_{1-x}F_xBiS_2$. The notable feature in $CeO_{1-x}F_xBiS_2$ is the observation of the magnetic ordering which was suggested to be a result of the ferromagnetic ordering of the Ce moment. Demura et al. showed that HP annealing can induce bulk superconductivity in $CeO_{1-x}F_xBiS_2$ as in the case of $LaO_{1-x}F_xBiS_2$ [33]. The T_c of the HP-annealed samples of $CeO_{1-x}F_xBiS_2$ obviously increases. The maximum T_c is 3K for the as grown samples and approximately 8K for the HP-annealed samples in the resistivity measurements [18]. Furthermore, the shielding volume fraction is also strongly enhanced in the HP-annealed samples, indicating the evolution of bulk superconducting states. Interestingly, the signals of the magnetic ordering of Ce still exist. Hence, the magnetic ordering at the CeO layer and the bulk superconducting states at the BiS_2 layers occur simultaneously in the HP sample. Although the magnetic structure of $CeO_{1-x}F_xBiS_2$ has not been clarified yet, it is clear that magnetism and superconductivity coexist in the HP-annealed $CeO_{1-x}F_xBiS_2$ samples.

The F concentration dependence of ferromagnetism and the superconducting transition temperature is shown in the phase diagrams of Figs.(2.11)(a) and (b) to understand the physical properties of the $CeO_{1-x}F_xBiS_2$ system [18]. From Fig.(2.11)(a), the ferromagnetic phases observed at 4.5K and 7.5K are given the terms lower temperature phase and higher temperature phase respectively. The lower temperature phase (4.5K) exists between x = 0.45 and 0.6, and coexists with the higher temperature phase (7.5 K) at x = 0.6. Above x = 0.6, the higher temperature phase (7.5K) can be observed. In Fig.(2.11)(b), the AG samples show superconductivity from x = 0.45 to 1.0. After high-pressure annealing, superconductivity appears in a large region between x = 0.3 and 1.0. The T_c of the HP samples is obviously higher than that of the AG samples.
Therefore, bulk superconductivity of $CeO_{1-x}F_xBiS_2$ could be induced with $x \geq 0.6$ in the HP samples. Interestingly, the F concentration where bulk superconductivity appears corresponds to the F concentration where the ferromagnetism with transition temperature of 7.5K.

Based on this experimental data, here we have to show the coexistence of ferromagnetism and bulk superconductivity in $CeO_{1-x}F_xBiS_2$ using double time temperature dependent Green's function.

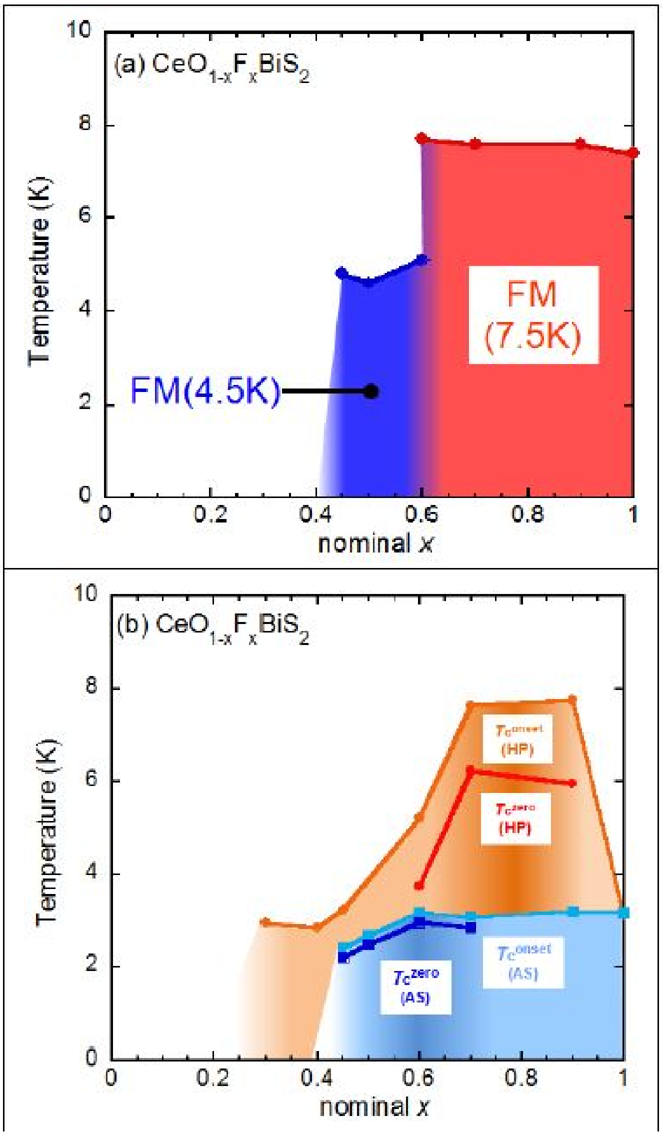

Figure 2.11: a) Phase diagram of magnetic ordering for the CeO blocking layers of HP-annealed $CeO_{1-x}F_xBiS_2$. b) Phase diagram of superconductivity with in the BiS_2 layers for HP-annealed $CeO_{1-x}F_xBiS_2$ [11, 18].

CHAPTER 3

Mathematical Method

3.1 Introduction

In this research work, we have used the double time temperature dependent Green's function formalism to obtain the expressions for superconducting transition temperature (T_c), magnetic ordering temperature (T_m), superconducting and magnetic ordering parameters (Δ) and (η) respectively.

The temperature dependent Green functions were introduced by Matsubara [34]. He considered many-particle system with the Hamiltonian $H = H_0 + V$ and observed a remarkable similarity that exists between the evaluation of the grand partition function of the system and the vacuum expectation of the so-called S-matrix in quantum field theory. In essence, Matsubara observed and exploited, to great advantage, formal similarities between the statistical operator $\exp(-\beta H)$ and the quantum-mechanical time-evolution operator $\exp(iHt)$. As a result, he introduced thermal (temperature-dependent) Green functions which we call now the Matsubara Green functions.

3.2 Double-time Temperature Dependent Green's Function Formalism

Double-time temperature-dependent Green's function is important part of the modern theory of superconductivity and many body problems [34]. This method permits formulation of the theory in a very transparent and convenient form and provides a powerful tool to solve more complicated many body problems in superconductivity, which is given by,

$$G_r(t-t') = << \hat{A}(t); \hat{B}(t') >>= -i\theta(t-t') < [\hat{A}(t); \hat{B}(t')] >_r \tag{3.1}$$

where $<< .... >>$ is abbreviated notation for the Green's function, $< ... >$ indicates that one should average over grand canonical ensemble. $\theta(t-t')$ is a Heaviside step functions. It is also called a unit step function whose values is zero for negative argument and one for positive argument.

i.e

$$\theta(t-t') = \begin{cases} 1 & t > t' \\ 0 & t < t' \end{cases}$$

$\hat{A}(t)$ and $\hat{B}(t')$ are operators in the Heisenberg representations. They are expressed in terms of a product of quantized functions (particle creation and annihilation operators), and can be expressed as,

$$\hat{A}(t) = \exp(i\hat{H}t)\hat{A}(0)\exp(-i\hat{H}t)$$

In order to obtain the equation of motion, we differentiate Eq.(3.1) with respect to time t and multiply it by "i" as,

$$i\frac{d}{dt}G_r(t-t') = i\frac{d}{dt}(-i\theta(t-t') < [\hat{A}(t);\hat{B}(t')] >)$$

$$= \frac{d}{dt}\theta(t-t') < [\hat{A}(t);\hat{B}(t')] > -i\theta(t-t') < [i\frac{d}{dt}\hat{A}(t);\hat{B}(t')] >$$

$$= \frac{d}{dt}\theta(t-t') < [\hat{A}(t);\hat{B}(t')] > -i\theta(t-t') << [\hat{A}(t),\hat{H}];\hat{B}(t') >>$$

$$i\frac{d}{dt}G_r(t-t') = \frac{d}{dt}\theta(t-t') < [\hat{A}(t);\hat{B}(t')] > + << [\hat{A}(t),\hat{H}];\hat{B}(t') >> \tag{3.2}$$

where, $i\hbar\frac{d}{dt}A\hat{(t)} = [A\hat{(t)},\hat{H}]$, for $\hbar = 1$, indicates the commutation or anti commutation.

$$[\hat{A}(t);\hat{B}(t')] = \hat{A}(t)\hat{B}(t') \pm \hat{B}(t')\hat{A}(t)$$

positive for Fermi operators and negative for Bose operators.

But we have the following relation,

$$\theta(t-t') = \int_t^{-\infty}\delta(t-t')dt$$

$$\frac{d}{dt}\theta(t-t') = \delta(t-t')$$

Thus, Eq.(3.2) can be written as,

$$i\frac{d}{dt}G_r(t-t') = \delta(t-t') < [\hat{A}(t);\hat{B}(t')] > + << [\hat{A}(t),\hat{H}];\hat{B}(t') >>$$

At $t > t', \delta(t-t') = 1$ therefore,

$$i\frac{d}{dt}G_r(t-t') =< [\hat{A}(t);\hat{B}(t')] > + << [\hat{A}(t),\hat{H}];\hat{B}(t') >> \tag{3.3}$$

Let $G_r(\omega)$ be the Fourier transform of $G_r(t-t')$. Then, we have,

$$G_r(t-t') = \int_{-\infty}^{\infty} G_r(\omega)\exp(-i\omega(t-t'))d\omega$$

$$G_r(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G_r(t-t')\exp(-i\omega(t-t'))d(t-t')$$

Using this, Eq.(3.3) becomes,

$$\omega G_r(\omega) =< [\hat{A}(t); \hat{B}(t')] > + << [\hat{A}(t), \hat{H}]; \hat{B}(t') >>$$

$$\omega << \hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{k'\uparrow} >>= \delta_{kk'} + << [\hat{a}_{k\uparrow}, \hat{H}], \hat{a}^{\dagger}_{k'\uparrow} >> \tag{3.4}$$

where, $\hat{a}_{k\uparrow}$ and $\hat{a}^{\dagger}_{k'\uparrow}$ are annihilation and creation operators respectively.

The BCS Hamiltonian is given by,

$$\hat{H} = \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma} \hat{a}_{p\sigma} - \sum_{pp'} V_{pp'} \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} \hat{a}_{p'\downarrow} \hat{a}_{-p'\uparrow} \tag{3.5}$$

$$\omega << \hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{k'\uparrow} >>= \delta_{kk'} + << [\hat{a}_{k\uparrow}, \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma} \hat{a}_{p\sigma}$$

$$- \sum_{pp'} V_{pp'} \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} \hat{a}_{p'\downarrow} \hat{a}_{-p'\uparrow}], \hat{a}^{\dagger}_{k'\uparrow} >>$$

But, we have the following relations,

$$[A, B \pm C] = [A, B] \pm [A, C]$$

$$[A, BC] = [A, B]C + B[A, C]$$

Using these relation, we can commute as follows,

$$[\hat{a}_{k\uparrow}, \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma} \hat{a}_{p\sigma}] = \sum_{p\sigma} \epsilon_p ([\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\sigma}] \hat{a}_{p\sigma} + \hat{a}^{\dagger}_{p\sigma} [\hat{a}_{k\uparrow}, \hat{a}_{p\sigma}])$$

If $p = k$ and $\sigma =\uparrow$, then

$$[\hat{a}_{k\uparrow}, \sum_{k} \epsilon_k \hat{a}^{\dagger}_{k\uparrow} \hat{a}_{k\uparrow}] = \sum_{k} \epsilon_k ([\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{k\uparrow}] \hat{a}_{k\uparrow} + \hat{a}^{\dagger}_{k\uparrow} [\hat{a}_{k\uparrow}, \hat{a}_{k\uparrow}]$$

But we have the following relation,

$$[\hat{a}_{k\uparrow}, \hat{a}_{k\uparrow}] = 0$$

$$[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{k\uparrow}] = \delta_{kk} = 1$$

Therefore, using this relation we have

$$[\hat{a}_{k\uparrow}, \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma} \hat{a}_{p\sigma}] = \sum_{k} \epsilon_k \hat{a}_{k\uparrow} \tag{3.6}$$

Similarly,

$$[\hat{a}_{k\uparrow}, - \sum_{pp'} V_{pp'} \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} \hat{a}_{p'\downarrow} \hat{a}_{-p'\uparrow}] = - \sum_{pp'} V_{pp'} ([\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow}] \hat{a}_{p'\downarrow} \hat{a}_{-p'\uparrow}$$

$$+\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}[\hat{a}_{k\uparrow},\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}])$$

But, $[\hat{a}_{k\uparrow},\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]=0$

$$[\hat{a}_{k\uparrow},-\sum_{pp'}V_{pp'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]=-\sum_{pp'}V_{pp'}([\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}]\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow})$$

$$=-\sum_{pp'}V_{pp'}([\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{p\uparrow}]\hat{a}^{\dagger}_{-p\downarrow}+\hat{a}^{\dagger}_{p\uparrow}[\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{-p\downarrow}])\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}$$

But, we have the following relation,

$$[\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{p\uparrow}]=\delta_{kp},\ if\ p=k,\ \delta_{pk}=1,[\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{-p\downarrow}]=\delta_{k,-p}\delta_{\uparrow\downarrow}=0$$

$$[\hat{a}_{k\uparrow},-\sum_{pp'}V_{pp'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]=-V_{kk'}\sum_{kk'}\hat{a}^{\dagger}_{-k\downarrow}\hat{a}_{k'\downarrow}\hat{a}_{-k'\uparrow} \tag{3.7}$$

Substituting Eqs.(3.6), (3.7) into Eq.(3.4) we have,

$$\omega<<\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>>=\delta_{kk'}+<<\sum_{k}\epsilon_k\hat{a}_{k\uparrow}-V_{kk'}\sum_{kk'}\hat{a}^{\dagger}_{-k\downarrow}\hat{a}_{k'\downarrow}\hat{a}_{-k'\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>>$$

$$\omega<<\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>>=1+\epsilon_k<<\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>>-V_{kk'}\sum_{kk'}<<\hat{a}^{\dagger}_{-k\downarrow}\hat{a}_{k'\downarrow}\hat{a}_{-k'\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>>$$

$$(\omega-\epsilon_k)<<\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>>=1-V_{kk'}\sum_{kk'}<<\hat{a}^{\dagger}_{-k\downarrow}\hat{a}_{k'\downarrow}\hat{a}_{-k'\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>> \tag{3.8}$$

In general, we have to write higher order Green's function into lower order Green's function by using the decoupling procedure or Wick's theorem as,

$$<<\hat{a}^{\dagger}_{-k\downarrow}\hat{a}_{k'\downarrow}\hat{a}_{-k'\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>>=<\hat{a}_{k'\downarrow}\hat{a}_{-k'\uparrow}><<\hat{a}^{\dagger}_{-k\downarrow}\hat{a}^{\dagger}_{k'\uparrow}>>$$

Using this, Eq.(3.8) can be written as,

$$(\omega-\epsilon_k)<<\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>>=1-V_{kk'}\sum_{kk'}<\hat{a}_{k'\downarrow}\hat{a}_{-k'\uparrow}><<\hat{a}^{\dagger}_{-k\downarrow}\hat{a}^{\dagger}_{k'\uparrow}>>$$

Now, let,

$$\Delta=V_{kk'}\sum_{kk'}<\hat{a}_{k'\downarrow}\hat{a}_{-k'\uparrow}>$$

$$(\omega-\epsilon_k)<<\hat{a}_{k\uparrow},\hat{a}^{\dagger}_{k'\uparrow}>>=1-\Delta<<\hat{a}^{\dagger}_{-k\downarrow}\hat{a}^{\dagger}_{k'\uparrow}>> \tag{3.9}$$

We can also obtain the equation of motion for $<<\hat{a}^{\dagger}_{-k\downarrow},\hat{a}^{\dagger}_{k'\uparrow}>>$

$$\omega<<\hat{a}^{\dagger}_{-k\downarrow},\hat{a}^{\dagger}_{k'\uparrow}>>=<<[\hat{a}^{\dagger}_{-k\downarrow},\hat{H}],\hat{a}^{\dagger}_{k'\uparrow}>> \tag{3.10}$$

$$[\hat{a}^{\dagger}_{-k\downarrow},\hat{H}]=[\hat{a}^{\dagger}_{-k\downarrow},\sum_{p\sigma}\epsilon_p\hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}-\sum_{pp'}V_{pp'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] \tag{3.11}$$

$$[\hat{a}^\dagger_{-k\downarrow}, \sum_{p\sigma} \epsilon_p \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}] = \sum_{p\sigma} \epsilon_p([\hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}])$$

$$= \sum_{p\sigma} \epsilon_p([\hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{p\sigma}]\hat{a}_{p\sigma} + \hat{a}^\dagger_{p\sigma}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{p\sigma}])$$

$$[\hat{a}^\dagger_{-k\downarrow}, \sum_{p\sigma} \epsilon_p \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}] = \sum_{p\sigma} \epsilon_p([\hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{p\sigma}]\hat{a}_{p\sigma} + \hat{a}^\dagger_{p\sigma}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{p\sigma}])$$

If $p = -k$ and $\sigma =\downarrow$, then, $[\hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{p\downarrow}] = 0$ and $[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{p\downarrow}] = \delta_{pp} = -1$, then, the above equation becomes

$$[\hat{a}^\dagger_{-k\downarrow}, \sum_{p\sigma} \epsilon_p \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}] = -\sum_{k} \epsilon_k \hat{a}^\dagger_{-k\downarrow} \tag{3.12}$$

Similarly,

$$[\hat{a}^\dagger_{-k\downarrow}, -\sum_{pp'} V_{pp'}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] = -\sum_{pp'} V_{pp'}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]$$

$$= -\sum_{pp'} V_{pp'}([\hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}]\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow} + \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}])$$

$$= -\sum_{pp'} V_{pp'}(\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}])$$

where, $[\hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}] = 0$

$$[\hat{a}^\dagger_{-k\downarrow}, -\sum_{pp'} V_{pp'}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] = -\sum_{pp'} V_{pp'}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}(\hat{a}_{p'\downarrow}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{-p'\uparrow}]$$

$$+[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{p'\downarrow}]\hat{a}_{-p'\uparrow})$$

If $p' = -k$, then,

$$[\hat{a}^\dagger_{-k\downarrow}, -\sum_{pp'} V_{pp'}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] = -V_{pp'}\sum_{k} \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{-k\downarrow}]\hat{a}_{k\uparrow}$$

$$[\hat{a}^\dagger_{-k\downarrow}, -\sum_{pp'} V_{pp'}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] = -V_{pp'}\sum_{k} \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{k\uparrow} \tag{3.13}$$

Substituting Eqs.(3.12), (3.13) into Eq.(3.10), we get,

$$\omega << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>= -\epsilon_k << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >> -V_{pp'}\sum_{k} << \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{k\uparrow}, \hat{a}^\dagger_{k'\uparrow} >>$$

$$(\omega + \epsilon_k) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>= -V_{pp'}\sum_{k} << \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{k\uparrow}, \hat{a}^\dagger_{k'\uparrow} >>$$

By using Wick's theorem

$$-V\sum_k << \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{k\uparrow}, \hat{a}^\dagger_{k'\uparrow} >>= -V_{pp'}\sum_k < \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow} ><< \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k'\uparrow} >>$$

$$\Delta^* = V_{pp'}\sum_k < \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow} >$$

In real quantity $\Delta^* = \Delta$, then

$$(\omega + \epsilon_k) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>= -\Delta << \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k'\uparrow} >> \tag{3.14}$$

But, from Eq.(3.9) we have,

$$<< \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k'\uparrow} >>= \frac{1}{\omega - \epsilon_k}(1 - \Delta << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>)$$

Hence, Eq.(3.14) becomes,

$$(\omega + \epsilon_k) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>= \frac{-\Delta}{\omega - \epsilon_k}(1 - \Delta << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>)$$

$$(\omega + \epsilon_k)((\omega - \epsilon_k) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>= -\Delta + \Delta^2 << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>$$

$$(\omega^2 - \epsilon_k^2 - \Delta^2) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>= -\Delta$$

$$<< \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>= \frac{-\Delta}{\omega^2 - \epsilon_k^2 - \Delta^2} \tag{3.15}$$

The superconducting order parameter (Δ) is also given by,

$$\Delta = \frac{V}{\beta}\sum_{k,n} << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow} >>= \frac{-V}{\beta}\sum_{k,n}\frac{\Delta}{\omega^2 - \epsilon_k^2 - \Delta^2} \tag{3.16}$$

By changing the summation into integration and by introducing the density of state $N(\epsilon)$ we have the following,

$$\sum_k \equiv \int d^3k = \int_{-\epsilon_f}^{\infty} d\epsilon N(\epsilon)$$

Thus, Eq.(3.16) can be written as,

$$\Delta = \frac{-V}{\beta}\sum_n \int_{-\epsilon_f}^{\infty} d\epsilon N(\epsilon)\frac{\Delta}{\omega^2 - \epsilon_k^2 - \Delta^2} \tag{3.17}$$

The attractive interaction is effective in the region $-\hbar\omega_D < \epsilon < \hbar\omega_D$ assuming the density of states does not vary over this region, then, Eq.(3.17) becomes,

$$1 = \frac{-V}{\beta}N(0)\sum_n \int_{-\hbar\omega D}^{\hbar\omega_D} d\epsilon \frac{1}{\omega^2 - \epsilon_k^2 - \Delta^2} \tag{3.18}$$

Now changing ω to $i\omega_n$ and $\omega_n = (2n+1)\frac{\pi}{\beta}$

$$\frac{1}{N(0)V} = \frac{-2}{\beta}\sum_n \int_0^{\hbar\omega_D} \frac{d\epsilon}{-\omega_n^2 - \epsilon_k^2 - \Delta^2}$$

But, $\omega_n^2 = (2n+1)^2\frac{\pi^2}{\beta^2}$

$$\frac{1}{N(0)V} = 2\sum_n \int_0^{\hbar\omega_D} \frac{d\epsilon}{\beta(2n+1)^2\frac{\pi^2}{\beta^2} + (\epsilon_k^2 + \Delta^2)\beta}$$

$$\frac{1}{N(0)V} = 2\sum_n \int_0^{\hbar\omega_D} \frac{\beta d\epsilon}{(2n+1)^2\pi^2 + (\epsilon_k^2 + \Delta^2)\beta^2} \tag{3.19}$$

Let, $x = (\epsilon_k^2 + \Delta^2)^{\frac{1}{2}}\beta$, and $N(0)V = \lambda$, then we get,

$$\frac{1}{\lambda} = 2\int_0^{\hbar\omega_D} \sum_n \frac{\beta d\epsilon}{(2n+1)^2\pi^2 + x^2} \tag{3.20}$$

Using the relation $\frac{1}{2x}tanh(\frac{x}{2}) = \sum_n \frac{1}{(2n+1)^2\pi^2+x^2}$, the above equation can be written as,

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_D} \frac{2\beta d\epsilon}{2\beta\sqrt{\epsilon_k^2 + \Delta^2}} \tanh(\beta\frac{\sqrt{\epsilon_k^2 + \Delta^2}}{2}) \tag{3.21}$$

When, Δ is very small,

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_D} d\epsilon\frac{1}{\epsilon}\tanh(\frac{\beta\epsilon}{2}) \tag{3.22}$$

Let, $\frac{\beta\epsilon}{2} = y \longrightarrow d\epsilon = \frac{2dy}{\beta}$, then, Eq.(3.22) becomes

$$\frac{1}{\lambda} = \int_0^{y} dy\frac{1}{y}\tanh(y) \tag{3.23}$$

Then, integrating Eq.(3.23) by part, and using $\beta = \frac{1}{k_B T_c}$ we get the BCS expression.

$$\frac{1}{\lambda} = ln(y)\tanh(y)|_0^y - \int_0^y \frac{ln(y)dy}{\cosh^2 y} \tag{3.24}$$

For low temperature, $\tanh(y) = \tanh(\frac{\beta\epsilon}{2}) = \tanh(\frac{\epsilon}{2k_B T_c}) = 1$

$$\frac{1}{\lambda} = ln(\frac{\hbar\omega_D}{2k_B T_c}) - ln(\frac{\pi}{4\gamma}) \tag{3.25}$$

where, γ is the Euler constant having the value of $\gamma = 1.78$ [35]. Then, Eq.(3.25) can be written as,

$$k_B T_c = 1.14\hbar\omega_D \exp(\frac{-1}{\lambda}) \tag{3.26}$$

CHAPTER 4

Formulation of The Problem

4.1 The Model-Hamiltonian

In this chapter we formulated the model Hamiltonian and study theoretically the interplay of superconductivity and ferromagnetism in superconductor $CeO_{1-x}FxBiS_2$. Now considering a system of exchange interaction which acts between the conduction and localized electrons and with in the frame of the BCS model the Hamiltonian of the system can be expressed as,

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4$$

where, $\hat{H}_1$ is the kinetic energy of the conduction electrons and electron-electron pairing interaction through phonon exchange Hamiltonian, and is given by,

$$\hat{H}_1 = \sum_{k\sigma} \epsilon_k \hat{a}^\dagger_{k\sigma}\hat{a}_{k\sigma} - \sum_{kk'} V_{kk'}\hat{a}^\dagger_{k\uparrow}\hat{a}^\dagger_{-k\downarrow}\hat{a}_{k'\downarrow}\hat{a}_{-k'\uparrow} \tag{4.1}$$

ϵ_k, is the one electron energy measured relative to the chemical potential. $V_{kk'}$, defines the matrix elements of the interaction potential. $\hat{a}^\dagger_{k\sigma}$ and $\hat{a}_{k\sigma}$ are creation and annihilation operators of an electron specified by the wave vector k and spin σ.
$\hat{H}_2$ is localized electrons energy given by,

$$\hat{H}_2 = \sum_{l\sigma} \epsilon_l \hat{b}^\dagger_{l\sigma}\hat{b}_{l\sigma} \tag{4.2}$$

$\hat{b}^\dagger_{l\sigma}$ and $\hat{b}_{l\sigma}$ are the creation and annihilation operators of localized electrons respectively.
$\hat{H}_3$ is the intra coulomb repulsion energy of localized electrons, given by,

$$\hat{H}_3 = U\sum_{l} \hat{n}_{l\uparrow}\hat{n}_{l\downarrow} \tag{4.3}$$

$\hat{H}_4$ is the interaction term between the conduction and localized electrons due to some unspecified mechanism, it is may be due to spin fluctuation, with coupling constant γ.

$$\hat{H}_4 = \sum_{pll'} \gamma_{ll'}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow} + hc \tag{4.4}$$

where, hc is the hermitian conjugate which is equal to $\sum_{pll'} \gamma'_{ll'}\hat{a}_{p\downarrow}\hat{a}_{-p\uparrow}\hat{b}^\dagger_{l\uparrow}\hat{b}^\dagger_{l'\uparrow}$

4.2 Equation of Motion

Inorder to obtain the equation of motion, we use the retarded double time temperature dependent Green's function, which is written as,

$$G_r(t-t') = -i\theta(t-t') < [\hat{A}(t);\hat{B}(t')] >$$

. Through differentiating this equation and taking Fourier transform we have the following.

$$\omega G_r(\omega) =< [\hat{A}(t);\hat{B}(t')] > + << [\hat{A}(t),\hat{H}];\hat{B}(t') >>$$

4.2.1 Equation of Motion For Conduction Electrons

The equation of motion for conduction electrons is given by,

$$\omega << \hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{k'\uparrow} >>_{\omega}= 1+ << [\hat{a}_{k\uparrow}, \hat{H}], \hat{a}^{\dagger}_{k'\uparrow} >>_{\omega}$$

$$\omega << \hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{k'\uparrow} >>_{\omega}= 1+ << [\hat{a}_{k\uparrow}, \hat{H}_1+\hat{H}_2+\hat{H}_3+\hat{H}_4], \hat{a}^{\dagger}_{k'\uparrow} >>_{\omega} \tag{4.5}$$

Now, let us evaluate the commutation relation separately.

$$[\hat{a}_{k\uparrow}, \hat{H}_1] = [\hat{a}_{k\uparrow}, \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma} - \sum_{pp'} V_{pp'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] \tag{4.6}$$

$$[\hat{a}_{k\uparrow}, \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}] = \sum_{p\sigma} \epsilon_p [\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}]$$

$$[\hat{a}_{k\uparrow}, \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}] = \sum_{p\sigma} \epsilon_p ([\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\sigma}]\hat{a}_{p\sigma} + \hat{a}^{\dagger}_{p\sigma}[\hat{a}_{k\uparrow}, \hat{a}_{p\sigma}])$$

where, p=k and $\sigma =\uparrow$ $[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\sigma}] = \delta_{kk}\delta_{\uparrow\uparrow} = 1$. Thus,

$$[\hat{a}_{k\uparrow}, \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}] = \sum_{k} \epsilon_k \hat{a}_{k\uparrow} \tag{4.7}$$

$$\begin{aligned}
-V_{pp'}\sum_{pp'}[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] &= -V_{pp'}\sum_{pp'}([\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}]\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow} \\
&\quad + \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}[\hat{a}_{k\uparrow}, \hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]) \\
&= -V_{pp'}\sum_{pp'}([\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow}]\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow} + \hat{a}^{\dagger}_{p\uparrow}[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{-p\downarrow}]\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}
\end{aligned}$$

If p=k, the last term is zero, and we get,

$$-V_{pp'}\sum_{pp'}[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] = -V_{p'}\sum_{p'}(\delta_{kk}\delta_{\uparrow\uparrow}\hat{a}^{\dagger}_{-k\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow})$$

$$= -V_{p'} \sum_{p'} \hat{a}^{\dagger}_{-k\downarrow} \hat{a}_{p'\downarrow} \hat{a}_{-p'\uparrow}$$

Therefore,

$$-V_{pp'} \sum_{pp'} [\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} \hat{a}_{p'\downarrow} \hat{a}_{-p'\uparrow}] = -V \sum_{p'} \hat{a}^{\dagger}_{-k\downarrow} \hat{a}_{p'\downarrow} \hat{a}_{-p'\uparrow} \tag{4.8}$$

Now, using Eqs.(4.7) and (4.8), Eq.(4.6) becomes,

$$[\hat{a}_{k\uparrow}, \hat{H}_1] = \epsilon_k \hat{a}_{k\uparrow} - V \sum_{p'} \hat{a}^{\dagger}_{-k\downarrow} \hat{a}_{p'\downarrow} \hat{a}_{-p'\uparrow} \tag{4.9}$$

Then, let us calculate the commutation with $\hat{H}_2$

$$[\hat{a}_{k\uparrow}, \hat{H}_2] = [\hat{a}_{k\uparrow}, \sum_{l\sigma} \epsilon_l \hat{b}^{\dagger}_{l\sigma} \hat{b}_{l\sigma}]$$

$$= \sum_{l\sigma} \epsilon_l [\hat{a}_{k\uparrow}, \hat{b}^{\dagger}_{l\sigma} \hat{b}_{l\sigma}]$$

$$= \sum_{l\sigma} \epsilon_l (\hat{b}^{\dagger}_{l\sigma} [\hat{a}_{k\uparrow}, \hat{b}_{l\sigma}] + [\hat{a}_{k\uparrow}, \hat{b}^{\dagger}_{l\sigma}] \hat{b}_{l\sigma})$$

$$[\hat{a}_{k\uparrow}, \hat{H}_2] = 0 \tag{4.10}$$

The commutation with $\hat{H}_3$ can be calculated as follows.

$$[\hat{a}_{k\uparrow}, \hat{H}_3] = [\hat{a}_{k\uparrow}, U \sum_{l} \hat{n}_{l\uparrow} \hat{n}_{l\downarrow}] = u \sum_{l} [\hat{a}_{k\uparrow}, \hat{n}_{l\uparrow} \hat{n}_{l\downarrow}]$$

$$= U \sum_{l} ([\hat{a}_{k\uparrow}, \hat{n}_{l\uparrow}] \hat{n}_{l\downarrow} + \hat{n}_{l\uparrow} [\hat{a}_{k\uparrow}, \hat{n}_{l\downarrow}])$$

$$U \sum_{l} ([\hat{a}_{k\uparrow}, \hat{b}^{\dagger}_{l\uparrow} \hat{b}_{l\uparrow}] \hat{b}^{\dagger}_{l\downarrow} \hat{b}_{l\downarrow} + \hat{b}^{\dagger}_{l\uparrow} \hat{b}_{l\uparrow} [\hat{a}_{k\uparrow}, \hat{b}^{\dagger}_{l\downarrow} \hat{b}_{l\downarrow}])$$

where, $\hat{n}_{l\uparrow} = \hat{b}^{\dagger}_{l\uparrow} \hat{b}_{l\uparrow}$ and $\hat{n}_{l\downarrow} = \hat{b}^{\dagger}_{l\downarrow} \hat{b}_{l\downarrow}$, then

$$[\hat{a}_{k\uparrow}, \hat{H}_3] = 0 \tag{4.11}$$

Lastly, the commutation with $\hat{H}_4$ can be calculated as,

$$[\hat{a}_{k\uparrow}, \hat{H}_4] = [\hat{a}_{k\uparrow}, \sum_{pll'} \gamma_{ll'} \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} \hat{b}_{l\uparrow} \hat{b}_{l'\uparrow} + hc]$$

$$= \sum_{pll'} \gamma_{ll'} ([\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} \hat{b}_{l\uparrow} \hat{b}_{l'\uparrow}] + [\hat{a}_{k\uparrow}, hc])$$

$$= \sum_{pll'} \gamma_{ll'} ([\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow}] \hat{b}_{l\uparrow} \hat{b}_{l'\uparrow} + \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} [\hat{a}_{k\uparrow}, \hat{b}_{l\uparrow} \hat{b}_{l'\uparrow}]) + 0$$

But, $[\hat{a}_{k\uparrow}, \hat{b}_{l\uparrow}\hat{b}_{l'\uparrow}] = 0$

$$[\hat{a}_{k\uparrow}, \hat{H}_4] = \sum_{pll'} \gamma_{ll'}([\hat{a}_{k\uparrow}, \hat{a}^\dagger_{p\uparrow}]\hat{a}^\dagger_{-p\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow} + \hat{a}^\dagger_{p\uparrow}[\hat{a}_{k\uparrow}, \hat{a}^\dagger_{-p\downarrow}]\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow})$$

$$= \sum_{pll'} \gamma_{ll'}(\delta_{kp}\hat{a}^\dagger_{-p\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow} + \hat{a}^\dagger_{p\uparrow}\delta_{k-p}\delta_{\uparrow\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow})$$

If $p = k$ then the above expression becomes,

$$[\hat{a}_{k\uparrow}, \hat{H}_4] = \sum_{ll'} \gamma_{ll'}\hat{a}^\dagger_{-k\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow} \tag{4.12}$$

Substituting Eqs.(4.9), (4.10), (4.11) and (4.12) into Eq.(4.5) we get,

$$\omega << \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>= 1+ << \epsilon_k\hat{a}_{k\uparrow} - V\sum_{p'} \hat{a}^\dagger_{-k\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow} + \sum_{ll'} \gamma_{ll'}\hat{a}^\dagger_{-k\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$= 1 + \epsilon_k << \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >> -V\sum_{p'} << \hat{a}^\dagger_{-k\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$+\sum_{ll'} \gamma_{ll'} << \hat{a}^\dagger_{-k\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$= 1 + \epsilon_k << \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >> -V\sum_{p'} < \hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow} >< < \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$+\sum_{ll'} \gamma_{ll'} < \hat{b}_{l\uparrow}\hat{b}_{l'\uparrow} >< < \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$(\omega - \epsilon_k) << \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>= 1 - V\sum_{p'} < \hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow} >< < \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$+\sum_{ll'} \gamma_{ll'} < \hat{b}_{l\uparrow}\hat{b}_{l'\uparrow} >< < \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>$$

Let, $\Delta = V\sum_{p'} < \hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow} >$ and $\eta = \sum_{ll'} \gamma_{ll'} < \hat{b}_{l\uparrow}\hat{b}_{l'\uparrow} >$

$$(\omega - \epsilon_k) << \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>= 1 - \Delta << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >> +\eta << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$<< \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>= \frac{1 - (\Delta - \eta) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>}{\omega - \epsilon_k} \tag{4.13}$$

where, Δ and η are superconducting and magnetic order parameters respectively.

Now, let us solve the equation of motion for $<< \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>$.

$$\omega << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>=<< [\hat{a}^\dagger_{-k\downarrow}, \hat{H}], \hat{a}^\dagger_{k\uparrow} >> \tag{4.14}$$

$$[\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}] = [\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_1] + [\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_2] + [\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_3] + [\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_4] \tag{4.15}$$

$$[\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_1] = [\hat{a}^{\dagger}_{-k\downarrow}, \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma} - \sum_{pp'} V_{pp'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]$$

$$= \sum_{p\sigma} \epsilon_p [\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}] - \sum_{pp'} V_{pp'}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]$$

$$\sum_{p\sigma} \epsilon_p [\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}] = \sum_{p\sigma} \epsilon_p ([\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\sigma}]\hat{a}_{p\sigma} + \hat{a}^{\dagger}_{p\sigma}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}_{p\sigma}])$$

$$= -\sum_{p\sigma} \epsilon_p (\hat{a}^{\dagger}_{p\sigma}\delta_{-kp}\delta_{\downarrow\downarrow})$$

If $p = -k$ and $\sigma = \downarrow$ then, the above expression becomes,

$$\sum_{p\sigma} \epsilon_p [\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}] = -\epsilon_{-k}\hat{a}^{\dagger}_{-k\downarrow} \tag{4.16}$$

Similarly,

$$-\sum_{pp'} V_{pp'}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] = -\sum_{pp'} V_{pp'}([\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}]\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}$$

$$+\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}])$$

$$= -\sum_{pp'} V_{pp'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}([\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}_{p'\downarrow}]\hat{a}_{-p'\uparrow} + \hat{a}_{p'\downarrow}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}_{-p'\uparrow}])$$

$$= -\sum_{pp'} V_{pp'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}(\delta_{-kp'}\delta_{\downarrow\downarrow}\hat{a}_{-p'\uparrow} + \hat{a}_{p'\downarrow}\delta_{-k-p'}\delta_{\downarrow\uparrow})$$

If $p' = -k$, then,

$$-\sum_{pp'} V_{pp'}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] = -\sum_{p} V_p\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{k\uparrow} \tag{4.17}$$

Then, using Eqs.(4.17), (4.16) into Eq. (4.15) we get,

$$[\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_1] = -\epsilon_{-k}\hat{a}^{\dagger}_{-k\downarrow} - \sum_{p} V_p\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{k\uparrow} \tag{4.18}$$

Now let us solve the commutation with $\hat{H}_2$.

$$[\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_2] = [\hat{a}^{\dagger}_{-k\downarrow}, \sum_{l} \epsilon_l \hat{b}^{\dagger}_{l\sigma}\hat{b}_{l\sigma}] = \sum_{l} \epsilon_l [\hat{a}^{\dagger}_{-k\downarrow}, \hat{b}^{\dagger}_{l\sigma}\hat{b}_{l\sigma}]$$

$$= \sum_{l} \epsilon_l ([\hat{a}^{\dagger}_{-k\downarrow}, \hat{b}^{\dagger}_{l\sigma}]\hat{b}_{l\sigma} + \hat{b}^{\dagger}_{l\sigma}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{b}_{l\sigma}])$$

$$[\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_2] = 0 \tag{4.19}$$

And,

$$[\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_3] = [\hat{a}^{\dagger}_{-k\downarrow}, U\sum_l \hat{n}_{l\uparrow}\hat{n}_{l\downarrow}] = U\sum_l [\hat{a}^{\dagger}_{-k\downarrow}, \hat{n}_{l\uparrow}\hat{n}_{l\downarrow}]$$

$$= U\sum_l ([\hat{a}^{\dagger}_{-k\downarrow}, \hat{n}_{l\uparrow}]\hat{n}_{l\downarrow} + \hat{n}_{l\uparrow}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{n}_{l\downarrow}])$$

$$[\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_3] = 0 \tag{4.20}$$

finally, the commutation with $\hat{H}_4$ can be calculated as follows,

$$[\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_4] = [\hat{a}^{\dagger}_{-k\downarrow}, \sum_{pll'} \gamma_{ll'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow} + hc]$$

$$[\hat{a}^{\dagger}_{-k\downarrow}, \hat{H}_4] = \sum_{pll'} \gamma_{ll'}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow}] + [\hat{a}^{\dagger}_{-k\downarrow}, hc] \tag{4.21}$$

$$\sum_{pll'} \gamma_{ll'}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow}] = \sum_{pll'} \gamma_{ll'}([\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}]\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow} + \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{b}_{l\uparrow}\hat{b}_{l'\uparrow}])$$

$$= \sum_{pll'} \gamma_{ll'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}([\hat{a}^{\dagger}_{-k\downarrow}, \hat{b}_{l\uparrow}]\hat{b}_{l'\uparrow} + \hat{b}_{l\uparrow}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{b}_{l'\uparrow}])$$

$$= \sum_{pll'} \gamma_{ll'}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{b}_{l\uparrow}\hat{b}_{l'\uparrow}] = 0 \tag{4.22}$$

Similarly,

$$[\hat{a}^{\dagger}_{-k\downarrow}, hc] = [\hat{a}^{\dagger}_{-k\downarrow}, \sum_{pll'} \gamma'_{ll'}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}\hat{b}^{\dagger}_{l\uparrow}\hat{b}^{+}_{l'\uparrow}] \tag{4.23}$$

where, hc is hermitian conjugate, which is equal to $\sum_{pll'} \gamma'_{ll'}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}\hat{b}^{\dagger}_{l\uparrow}\hat{b}^{+}_{l'\uparrow}$.

$$[\hat{a}^{\dagger}_{-k\downarrow}, hc] = \sum_{pll'} \gamma'_{ll'}([\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}]\hat{b}^{\dagger}_{l\uparrow}\hat{b}^{\dagger}_{l'\uparrow} + \hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{b}^{\dagger}_{l\uparrow}\hat{b}^{\dagger}_{l'\uparrow}])$$

$$= \sum_{pll'} \gamma'_{ll'}([\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}_{p\uparrow}]\hat{a}_{-p\downarrow} + \hat{a}_{p\uparrow}[\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}_{-p\downarrow}])\hat{b}^{\dagger}_{l\uparrow}\hat{b}^{\dagger}_{l'\uparrow}$$

$$= \sum_{pll'} \gamma'_{ll'}(\delta_{-kp}\sigma_{\downarrow\uparrow}\hat{a}_{-p\downarrow} + \hat{a}_{p\uparrow}\delta_{-k-p})\hat{b}^{\dagger}_{l\uparrow}\hat{b}^{\dagger}_{l'\uparrow}$$

But, $\sigma_{\downarrow\uparrow} = 0$ and if p=k, then,

$$[\hat{a}^{\dagger}_{-k\downarrow}, hc] = \sum_{ll'} \gamma'_{ll'}\hat{a}_{k\uparrow}\hat{b}^{\dagger}_{l\uparrow}\hat{b}^{\dagger}_{l'\uparrow} \tag{4.24}$$

Therefore, using Eqs.(4.22) and (4.24) into Eq. (4.21) we get,

$$[\hat{a}^\dagger_{-k\downarrow}, \hat{H}_4] = \sum_{ll'} \gamma'_{ll'} \hat{a}_{k\uparrow} \hat{b}^\dagger_{l\uparrow} \hat{b}^\dagger_{l'\uparrow} \tag{4.25}$$

Then, using Eqs.(4.18), (4.19), (4.20) and (4.25) into Eq. (4.14) we get,

$$\omega << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>=<< -\epsilon_{-k}\hat{a}^\dagger_{-k\downarrow} - \sum_p V_p \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{k\uparrow} + \sum_{ll'} \gamma'_{ll'}\hat{a}_{k\uparrow}\hat{b}^\dagger_{l\uparrow}\hat{b}^\dagger_{l'\uparrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$= -\epsilon_{-k} << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >> - \sum_p V_p << \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$+ \sum_{ll'} \gamma'_{ll'} << \hat{a}_{k\uparrow}\hat{b}^\dagger_{l\uparrow}\hat{b}^\dagger_{l'\uparrow}, \hat{a}^\dagger_{k\uparrow} >>$$

By using Wick's theorem or decoupling procedure we can write the higher order Green's function into lower order Green's function as follows.

$$\omega << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>= -\epsilon_{-k} << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >> - \sum_p V_p < \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow} ><< \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$+ \sum_{ll'} \gamma'_{ll'} < \hat{b}^\dagger_{l\uparrow}\hat{b}^\dagger_{l'\uparrow} ><< \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>$$

Let, $\Delta^* = \sum_p V_p < \hat{a}^\dagger_{p\uparrow}, \hat{a}^\dagger_{-p\downarrow} >$ and $\eta^* = \sum_{ll'} \gamma'_{ll'} < \hat{b}^\dagger_{l\uparrow}, \hat{b}^\dagger_{l'\uparrow} >$, Since energy and order parameters are real, they are equal to Δ and η respectively. For $\epsilon_{-k} = \epsilon_k$, we have,

$$(\omega + \epsilon_k) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>= -(\Delta - \eta) << \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>$$

$$<< \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>= \frac{-(\Delta - \eta) << \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>}{\omega + \epsilon_k} \tag{4.26}$$

But from Eq.(4.13) we have,

$$<< \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k\uparrow} >>= \frac{1 - (\Delta - \eta) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>}{\omega - \epsilon_k}$$

Thus, Eq.(4.26) becomes,

$$<< \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>= (\frac{-(\Delta - \eta)}{\omega + \epsilon_k})(\frac{1 - (\Delta - \eta) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>}{\omega - \epsilon_k})$$

$$<< \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>= \frac{-(\Delta - \eta)}{\omega^2 - \epsilon_k^2}(1 - (\Delta - \eta) << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>)$$

$$<< \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>= \frac{-(\Delta - \eta)}{\omega^2 - \epsilon_k^2} + \frac{(\Delta - \eta)^2}{\omega^2 - \epsilon_k^2} << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>$$

Solving for $<< \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>$, we get,

$$<< \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >>= \frac{-(\Delta-\eta)}{\omega^2-\epsilon_k^2-(\Delta-\eta)^2} \tag{4.27}$$

This is the required equation of motion for conduction electrons. Taking into account the temperature dependence of superconducting order parameter (Δ), we can write it as,

$$\Delta = \frac{V}{\beta}\sum_{k,n} << \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow} >> \tag{4.28}$$

where, the summation over k and n includes all order pairs and $\beta = \frac{1}{k_B T}$. Thus, using Eq.(4.27) in Eq.(4.28), we get,

$$\Delta = \frac{-V}{\beta}\sum_{k,n}\frac{(\Delta-\eta)}{\omega^2-\epsilon_k^2-(\Delta-\eta)^2} \tag{4.29}$$

The summation over k can be changed into integration by introducing the density of state $N(\epsilon)$.

$$\sum_k \longrightarrow \int d^3K = \int_{-\epsilon_f}^{\infty} d\epsilon N(\epsilon)$$

By using the above relation, Eq.(4.29) becomes,

$$\Delta = \frac{-V}{\beta}\sum_{n}\int_{-\epsilon_f}^{\infty} d\epsilon N(\epsilon)\frac{(\Delta-\eta)}{\omega^2-\epsilon_k^2-(\Delta-\eta)^2} \tag{4.30}$$

Using $\omega = i\omega_n \longrightarrow \omega^2 = -\omega_n^2$, where Matsubara frequency $\omega_n = (2n+1)\frac{\pi}{\beta}$ Eq. (4.30) can be written as,

$$\Delta = \frac{-V}{\beta}\sum_{n}\int_{-\epsilon_f}^{\infty} d\epsilon N(\epsilon)\frac{(\Delta-\eta)}{-\omega_n^2-(\epsilon_k^2+(\Delta-\eta)^2)}$$

$$\Delta = \frac{-V}{\beta}\sum_{n}\int_{-\epsilon_f}^{\infty} d\epsilon N(\epsilon)\frac{(\Delta-\eta)}{-(2n+1)^2\frac{\pi^2}{\beta^2}-(\epsilon_k^2+(\Delta-\eta)^2)}$$

$$\Delta = V\beta\sum_{n}\int_{-\epsilon_f}^{\infty} d\epsilon N(\epsilon)\frac{(\Delta-\eta)}{(2n+1)^2\pi^2+(\epsilon_k^2+(\Delta-\eta)^2)\beta^2}$$

$$\Delta = V\beta\sum_{n}\int_{-\epsilon_f}^{\infty} d\epsilon N(\epsilon)\frac{(\Delta-\eta)}{(2n+1)^2\pi^2+E^2\beta^2} \tag{4.31}$$

where, $E^2 = \epsilon_k^2 + (\Delta-\eta)^2$
Since the attractive interaction of electrons are effective in the region $-\hbar\omega_b < \epsilon < \hbar\omega_b$, and using the density of state is constant in this region, Eq.(4.31) becomes,

$$\Delta = 2V\beta N(0)\sum_n \int_0^{\hbar\omega_b} \frac{(\Delta-\eta)}{(2n+1)^2\pi^2 + E^2\beta^2} d\epsilon \tag{4.32}$$

Using the relation $\frac{1}{2x}tanh(\frac{x}{2}) = \sum_n \frac{1}{(2n+1)^2\pi^2+x^2}$, where, $x = \beta E$ Eq.(4.32) can be written as,

$$\Delta = 2V\beta N(0)\int_0^{\hbar\omega_b} \frac{(\Delta-\eta)}{2\beta E}\tanh(\frac{\beta E}{2})d\epsilon$$

$$\Delta = VN(0)\int_0^{\hbar\omega_b} \frac{(\Delta-\eta)}{E}\tanh(\frac{\beta E}{2})d\epsilon \tag{4.33}$$

Let, $VN(0) = \lambda$ and is the superconducting coupling parameter. Thus, Eq.(4.33) becomes,

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega_b} \frac{(\Delta-\eta)}{\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}\tanh(\frac{\beta\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}{2})d\epsilon \tag{4.34}$$

Now, let us study the properties of Eq.(4.34) by considering different cases.

Case I: When $T \longrightarrow 0$, $\beta = \frac{1}{k_BT} \longrightarrow \infty$, so that, $\tanh(\frac{\beta\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}{2}) = 1$. Hence Eq.(4.34) becomes,

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega_b} \frac{(\Delta-\eta)}{\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}d\epsilon \tag{4.35}$$

Now, using the relation $\int \frac{a}{\sqrt{a^2+x^2}}dx = a\sinh^{-1}(\frac{x}{a})$ Eq.(4.35) can be written as,

$$\frac{\Delta}{\lambda} = (\Delta-\eta)\sinh^{-1}(\frac{\epsilon}{(\Delta-\eta)})|_0^{\hbar\omega_b} \tag{4.36}$$

$$\frac{1}{\lambda} = (1-\frac{\eta}{\Delta})\sinh^{-1}(\frac{\hbar\omega_b}{(\Delta-\eta)})$$

$$\frac{1}{\lambda} \approx (1-\frac{\eta}{\Delta})ln(\frac{2\hbar\omega_b}{\Delta-\eta}) \tag{4.37}$$

Solving for $(\Delta-\eta)$ we get,

$$\Delta-\eta = 2\hbar\omega_b exp(\frac{-1}{\lambda(1-\frac{\eta}{\Delta})}) \tag{4.38}$$

But, from the BCS theory at $T = 0$ we have $\Delta \approx 1.75k_BT_c$. For $CeO_{1-x}F_xBiS_2$ superconductor the experimental value of the transition temperature, $T_c \approx 8K$ [18], so that $\Delta(0) \approx 19.329x10^{-23}J$, and the value of k_B(Boltzmann constant)$= 1.38065x10^{-23}J/K$.

$$1.75k_BT_c - \eta = 2\hbar\omega_b exp(\frac{-1}{\lambda(1-\frac{\eta}{\Delta})})$$

$$\eta = 1.75k_BT_c - 2\hbar\omega_b exp(\frac{-1}{\lambda(1-\frac{\eta}{1.75k_BT_c})}) \tag{4.39}$$

It is vital to note that Eq.(4.39) reduces to the BCS model for $\eta = 0$.

Case II: For $T \longrightarrow T_c$ $\Delta(T) = 1.76\Delta(0)\sqrt{(1-\frac{T}{T_c})} \longrightarrow 0$. Thus, using Eq.(4.34), we get

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega_b} \frac{(\Delta-\eta)}{\sqrt{\epsilon_k^2+(\Delta-\eta)^2}} \tanh(\frac{\beta\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}{2})d\epsilon \tag{4.40}$$

$$\frac{1}{\lambda} = (1-\frac{\eta}{\Delta})\int_0^{\hbar\omega_b} \frac{1}{\sqrt{\epsilon_k^2+(\Delta-\eta)^2}} \tanh(\frac{\beta\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}{2})d\epsilon$$

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} \frac{1}{\sqrt{\epsilon_k^2+(\Delta-\eta)^2}} \tanh(\frac{\beta\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}{2})d\epsilon$$

$$- \int_0^{\hbar\omega_b} \frac{\eta}{\Delta\sqrt{\epsilon_k^2+(\Delta-\eta)^2}} \tanh(\frac{\beta\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}{2})d\epsilon \tag{4.41}$$

Integral of the first expression (let's say I_1) of Eq.(4.41) at $T = T_c$, $\Delta = 0$, becomes

$$I_1 = \int_0^{\hbar\omega_b} \frac{1}{\sqrt{\epsilon_k^2+\eta^2}} \tanh(\frac{\beta\sqrt{\epsilon_k^2+\eta^2}}{2})d\epsilon = \int_0^{\hbar\omega_b} \frac{2\beta}{2\beta\sqrt{\epsilon_k^2+\eta^2}} \tanh(\frac{\beta\sqrt{\epsilon_k^2+\eta^2}}{2})d\epsilon$$

Using the relation $\frac{1}{2x}\tanh(\frac{x}{2}) = \sum_n \frac{1}{(2n+1)^2\pi^2+x^2}$ and $\omega_n = (2n+1)\frac{\pi}{\beta}$ the above equation becomes,

$$I_1 = \int_0^{\hbar\omega_b} d\epsilon \frac{2}{\beta}\sum_{n=-\infty}^{\infty} \frac{1}{\omega_n^2+\epsilon_k^2+\eta^2}$$

where, $x = \beta\sqrt{\epsilon_k^2+\eta^2}$

Taking Laplace transformation and Matsubara frequency (ω_n), the above integral becomes,

$$I_1 = \int_0^{\hbar\omega_b} \frac{1}{\epsilon}\tanh(\frac{\beta\epsilon}{2})d\epsilon - \int_0^{\hbar\omega_b} \eta^2\frac{2}{\beta}\sum_{-\infty}^{\infty} \frac{1}{(((2n+1)\frac{\pi}{\beta})^2+\epsilon^2)^2}d\epsilon + ... \tag{4.42}$$

Since, $\sum_{-\infty}^{\infty} \frac{1}{(((2n+1)\frac{\pi}{\beta})^2+\epsilon^2)^2} = 2\sum_0^{\infty} \frac{1}{(((2n+1)\frac{\pi}{\beta})^2+\epsilon^2)^2} = 2\sum_0^{\infty}\frac{1}{(a^2+\epsilon^2)^2} = 2\sum_0^{\infty}\frac{1}{a^4(1+\frac{\epsilon^2}{a^2})^2}$ where $a = (2n+1)\frac{\pi}{\beta}$, then

$$I_1 = \int_0^{\hbar\omega_b} \frac{1}{\epsilon}\tanh(\frac{\beta\epsilon}{2})d\epsilon - \int_0^{\hbar\omega_b} \eta^2\frac{4}{\beta}\sum_0^{\infty}\frac{1}{a^4(1+\frac{\epsilon^2}{a^2})^2}d\epsilon + ... \tag{4.43}$$

For $y=\frac{\beta\epsilon}{2}$, then

$$\int_0^{\hbar\omega_b}\frac{1}{\epsilon}\tanh(\frac{\beta\epsilon}{2})d\epsilon=\int_0^{\hbar\omega_b}\frac{1}{\frac{2y}{\beta}}\tanh(y)\frac{2}{\beta}dy=\int_0^{\hbar\omega_b}\frac{1}{y}\tanh(y)dy$$

$$=ln(y)\tanh(y)|_0^y-\int_0^y\frac{lny}{cosh^2y}dy$$

For low temperature, $tanh(y)=tanh(\frac{\beta\epsilon}{2})=tanh(\frac{\hbar\omega_b}{2k_BT})\longrightarrow 1$, then,

$$\int_0^{\hbar\omega_b}\frac{1}{\epsilon}\tanh(\frac{\beta\epsilon}{2})d\epsilon=ln(\frac{\hbar\omega_b}{2k_BT})-ln(\frac{\pi}{4\gamma})$$

where γ is the Euler constant having the value $\gamma=1.78$ [35], then, the above equation becomes,

$$\int_0^{\hbar\omega_b}\frac{1}{\epsilon}\tanh(\frac{\beta\epsilon}{2})d\epsilon=ln(1.14\frac{\hbar\omega_b}{k_BT_c})\tag{4.44}$$

And, let $x=\frac{\epsilon}{a}\longrightarrow d\epsilon=adx$

$$\int_0^{\hbar\omega_b}\eta^2\frac{4}{\beta}\sum_0^{\infty}\frac{1}{a^4(1+\frac{\epsilon^2}{a^2})^2}d\epsilon+...=\frac{4\eta^2}{\beta}\sum_0^{\infty}\int_0^{\infty}\frac{adx}{a^4(1+x^2)^2}+...\tag{4.45}$$

$$=\frac{4\eta^2}{\beta}\sum_0^{\infty}\int_0^{\infty}\frac{dx}{((2n+1)\frac{\pi}{\beta})^3(1+x^2)^2}$$

$$=\frac{4\eta^2\beta^2}{\pi^3}\sum_0^{\infty}\frac{1}{(2n+1)^3}\int_0^{\infty}\frac{dx}{(1+x^2)^2}$$

But, $\int_0^{\infty}\frac{dx}{(1+x^2)^2}=\frac{\pi}{4}$ and $\sum_0^{\infty}\frac{1}{(2n+1)^n}=(1-2^{-n})\zeta(n)$, here, $n=3$, $\sum_0^{\infty}\frac{1}{(2n+1)^3}=(1-2^{-3})\zeta(3)$ where, ζ is zeta function $\zeta(3)=1.202$, on using all this we get,

$$\int_0^{\hbar\omega_b}\eta^2\frac{4}{\beta}\sum_0^{\infty}\frac{1}{a^4(1+\frac{\epsilon^2}{a^2})^2}d\epsilon+...=\frac{4\eta^2\beta^2}{\pi^3}(1-2^{-3})\zeta(3)\frac{\pi}{4}\tag{4.46}$$

$$=\frac{\eta^2\beta^2}{\pi^2}*\frac{7}{8}*1.202$$

$$=(\frac{\eta}{\pi k_BT_c})^2(\frac{8.414}{8})\tag{4.47}$$

Thus, using Eq.(4.44) and Eq.(4.47) into Eq.(4.43), we get,

$$I_1=ln(1.14\frac{\hbar\omega_b}{k_BT_c})-(\frac{\eta}{\pi k_BT_c})^2(\frac{8.414}{8})\tag{4.48}$$

Then, let us integrate the second exasperation(say I_2) of Eq.(4.41) by applying L'Hopital's Rule

$$I_2=\int_0^{\hbar\omega_b}\lim_{\Delta\longrightarrow 0}\frac{\eta}{\Delta\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}\tanh(\frac{\beta\sqrt{\epsilon_k^2+(\Delta-\eta)^2}}{2})d\epsilon$$

$$I_2 = \int_0^{\hbar\omega_b} \lim_{\Delta \longrightarrow 0} \eta \frac{sech^2(\frac{\beta\sqrt{\epsilon^2+(\Delta-\eta)^2}}{2})\frac{\beta(\Delta-\eta)}{2\sqrt{\epsilon^2+(\Delta-\eta)^2}}}{\sqrt{\epsilon^2+(\Delta-\eta)^2}+\frac{\Delta(\Delta-\eta)}{\sqrt{\epsilon^2+(\Delta-\eta)^2}}} d\epsilon$$

$$I_2 = -\int_0^{\hbar\omega_b} \frac{\eta^2 \beta sech^2(\frac{\beta}{2}\sqrt{\epsilon^2+\eta^2})}{2\sqrt{\epsilon^2+\eta^2}} d\epsilon \tag{4.49}$$

Therefore, using Eq.(4.48) and Eq.(4.49) into Eq.(4.41) we have,

$$\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_B T_c}) - (\frac{\eta}{\pi k_B T_c})^2 \frac{8.414}{8} + \int_0^{\hbar\omega_b} \frac{\eta^2 \beta sech^2(\frac{\beta}{2}\sqrt{\epsilon^2+\eta^2})}{2\sqrt{\epsilon^2+\eta^2}} d\epsilon$$

Using the relation $sech^2 x = 1 - tanh^2 x$, we can write

$$\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_B T_c}) - (\frac{\eta}{\pi k_B T_c})^2 \frac{8.414}{8} + \int_0^{\hbar\omega_b} \frac{\eta^2}{2k_B T_c\sqrt{\epsilon^2+\eta^2}} d\epsilon$$

$$- \int_0^{\hbar\omega_b} \frac{\eta^2 tanh^2(\frac{\beta}{2}\sqrt{\epsilon^2+\eta^2})}{2k_B T_c\sqrt{\epsilon^2+\eta^2}} d\epsilon$$

where, $\int_0^{\hbar\omega_b} \frac{\eta^2}{2k_B T_c\sqrt{\epsilon^2+\eta^2}} d\epsilon = \frac{\eta^2 tanh^{-1}(\frac{\hbar\omega_b}{\eta})}{2k_B T_c} = \frac{\eta}{4k_B T_c} ln(\frac{\eta+\hbar\omega_b}{\eta-\hbar\omega_b})$.

And the fourth term can be integrated using the help of Fortran language and using the approximation $\hbar\omega_b = \hbar\omega_D = 10^{-3}ev$(for BCS), then we get the following expression.

$$\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_B T_c}) + \frac{\eta}{4k_B T_c} ln(\frac{\eta+\hbar\omega_b}{\eta-\hbar\omega_b}) - \frac{\eta^2}{(\pi k_B T_c)^2}\frac{8.414}{8} - \frac{7.5x10^{-19}\eta^2}{(2k_B T_c)^2}$$

For small η we can ignore the η^2 term of the above equation, and obtain,

$$\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_B T_c}) + \frac{\eta}{4k_B T_c} ln(\frac{\eta+\hbar\omega_b}{\eta-\hbar\omega_b}) \tag{4.50}$$

Let, $a = \frac{1}{4k_B T_c} ln(\frac{\eta+\hbar\omega_b}{\eta-\hbar\omega_b})$, then Eq.(4.50) becomes,

$$\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_B T_c}) + \eta a \tag{4.51}$$

Solving for T_c we get,

$$T_c = 1.14\frac{\hbar\omega_b}{k_B} e^{-(\frac{1}{\lambda}-\eta a)} \tag{4.52}$$

4.2.2 Equation of Motion For Localized Electrons

The equation of motion for localized electrons can be obtained by using retarded double time temperature Green's function formalism as follow.

$$\omega << \hat{b}_{l\uparrow}, \hat{b}^\dagger_{l\uparrow} >>_w = 1 + << [\hat{b}_{l\uparrow}, \hat{H}], \hat{b}^\dagger_{l\uparrow} >>_\omega \tag{4.53}$$

First, let us evaluate the commutation with the Hamiltonian ($[\hat{b}_{l\uparrow}, \hat{H}]) = [\hat{b}_{l\uparrow}, \hat{H}_1] + [\hat{b}_{l\uparrow}, \hat{H}_2] + [\hat{b}_{l\uparrow}, \hat{H}_3] + [\hat{b}_{l\uparrow}, \hat{H}_4]$

$$[\hat{b}_{l\uparrow}, \hat{H}_1] = [\hat{b}_{l\uparrow}, \sum_{p,\sigma} \epsilon_p \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma} - \sum_{p,p'} V(pp')\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}] \tag{4.54}$$

$$= \sum_{p,\sigma} \epsilon_p [\hat{b}_{l\uparrow}, \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}] - \sum_{p,p'} V(p,p')[\hat{b}_{l\uparrow}, \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]$$

$$[\hat{b}_{l\uparrow}, \hat{H}_1] = 0 \tag{4.55}$$

Applying the same procedure the commutation with $\hat{H}_2$ ($[\hat{b}_{l\uparrow}, \hat{H}_2]$) can be solved as follow

$$[\hat{b}_{l\uparrow}, \hat{H}_2] = [\hat{b}_{l\uparrow}, \sum_m \epsilon_m \hat{b}^\dagger_{m\sigma}\hat{b}_{m\sigma}] = \sum_m \epsilon_m [\hat{b}_{l\uparrow}, \hat{b}^\dagger_{m\sigma}\hat{b}_{m\sigma}]$$

$$= \sum_m \epsilon_m ([\hat{b}_{l\uparrow}, \hat{b}^+_{m\sigma}]\hat{b}_{m\sigma} + \hat{b}^\dagger_{m\sigma}[\hat{b}_{l\uparrow}, \hat{b}_{m\sigma}]) \tag{4.56}$$

$$= \sum_m \epsilon_m (\delta_{lm}\delta_{\uparrow\sigma}\hat{b}_{m\sigma}) \tag{4.57}$$

If $m = l$ and $\sigma =\uparrow$, then we get,

$$[\hat{b}_{l\uparrow}, \hat{H}_2] = \epsilon_l \hat{b}_{l\uparrow} \tag{4.58}$$

The commutation with intra Coulomb repulsion interaction Hamiltonian ($\hat{H}_3$) can be calculated as follow.

$$[\hat{b}_{l\uparrow}, \hat{H}_3] = [\hat{b}_{l\uparrow}, U\sum_m \hat{n}_{m\uparrow}\hat{n}_{m\downarrow}] = U\sum_m [\hat{b}_{l\uparrow}, \hat{n}_{m\uparrow}\hat{n}_{m\downarrow}]$$

$$= U\sum_m ([\hat{b}_{l\uparrow}, \hat{n}_{m\uparrow}]\hat{n}_{m\downarrow} + \hat{n}_{m\uparrow}[\hat{b}_{l\uparrow}, \hat{n}_{m\downarrow}])$$

$$= U\sum_m ([\hat{b}_{l\uparrow}, \hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}]\hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow} + \hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}[\hat{b}_{l\uparrow}, \hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow}])$$

where, $\hat{n}_{m\uparrow} = \hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}$ and $\hat{n}_{m\downarrow} = \hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow}$

$$[\hat{b}_{l\uparrow}, \hat{H}_3] = U\sum_m ([\hat{b}_{l\uparrow}, \hat{b}^\dagger_{m\uparrow}]\hat{b}_{m\uparrow}\hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow} + \hat{b}^\dagger_{m\uparrow}[\hat{b}_{l\uparrow}, \hat{b}_{m\uparrow}]\hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow}$$

$$+\hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}[\hat{b}_{l\uparrow}, \hat{b}^\dagger_{m\downarrow}]\hat{b}_{m\downarrow} + \hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}\hat{b}^\dagger_{m\downarrow}[\hat{b}_{l\uparrow}, \hat{b}_{m\downarrow}])$$

$$= U\sum_m [\hat{b}_{l\uparrow}, \hat{b}^\dagger_{m\uparrow}]\hat{b}_{m\uparrow}\hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow}$$

$$= U\sum_m \delta_{lm}\delta_{\uparrow\uparrow}\hat{b}_{m\uparrow}\hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow}$$

$$[\hat{b}_{l\uparrow}, \hat{H}_3] = U\hat{b}_{l\uparrow}\hat{b}^{\dagger}_{l\downarrow}\hat{b}_{l\downarrow} \tag{4.59}$$

where, $m = l$
Similarly, the commutation with $\hat{H}_4$ becomes,

$$[\hat{b}_{l\uparrow}, \hat{H}_4] = [\hat{b}_{l\uparrow}, \sum_{p,m,l'} \gamma_{ml'}\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{b}_{m\uparrow}\hat{b}_{l'\uparrow} + hc]$$

$$= \sum_{p,m,l'} \gamma_{ml'}[\hat{b}_{l\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{b}_{m\uparrow}\hat{b}_{l'\uparrow}] + [\hat{b}_{l\uparrow}, hc]$$

Now, let us commute separately,

$$\sum_{p,m,l'} \gamma_{ml'}[\hat{b}_{l\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{b}_{m\uparrow}\hat{b}_{l'\uparrow}] = \sum_{p,m,l'} \gamma_{ml'}([\hat{b}_{l\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}]\hat{b}_{m\uparrow}\hat{b}_{l'\uparrow}$$

$$+\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}[\hat{b}_{l\uparrow}, \hat{b}_{m\uparrow}\hat{b}_{l'\uparrow}])$$

$$= \sum_{p,m,l'} \gamma_{ml'}([\hat{b}_{l\uparrow}, \hat{a}^{\dagger}_{p\uparrow}]\hat{a}^{\dagger}_{-p\downarrow}\hat{b}_{m\uparrow}\hat{b}_{l'\uparrow} + \hat{a}^{\dagger}_{p\uparrow}[\hat{b}_{l\uparrow}, \hat{a}^{\dagger}_{-p\downarrow}]\hat{b}_{m\uparrow}\hat{b}_{l'\uparrow})$$

$$\sum_{p,m,l'} \gamma_{ml'}[\hat{b}_{l\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{b}_{m\uparrow}\hat{b}_{l'\uparrow}] = 0 \tag{4.60}$$

And

$$[\hat{b}_{l\uparrow}, hc] = [\hat{b}_{l\uparrow}, \sum_{p,m,l'} \gamma^{*}_{ml'}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}\hat{b}^{\dagger}_{m\uparrow}\hat{b}^{\dagger}_{l'\uparrow}] = \sum_{p,m,l'} \gamma^{*}_{ml'}[\hat{b}_{l\uparrow}, \hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}\hat{b}^{\dagger}_{m\uparrow}\hat{b}^{\dagger}_{l'\uparrow}]$$

$$= \sum_{p,m,l'} \gamma^{*}_{ml'}(\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}[\hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{m\uparrow}\hat{b}^{\dagger}_{l'\uparrow}] + [\hat{b}_{l\uparrow}, \hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}]\hat{b}^{\dagger}_{m\uparrow}\hat{b}^{\dagger}_{l'\uparrow})$$

$$= \sum_{p,m,l'} \gamma^{*}_{ml'}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}([\hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{m\uparrow}]\hat{b}^{\dagger}_{l'\uparrow} + \hat{b}^{\dagger}_{m\uparrow}[\hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l'\uparrow}])$$

$$= \sum_{p,m,l'} \gamma^{*}_{ml'}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}(\delta_{lm}\delta_{\uparrow\uparrow}\hat{b}^{\dagger}_{l'\uparrow} + \hat{b}^{\dagger}_{m\uparrow}\delta_{ll'}\delta_{\uparrow\uparrow})$$

$$= \sum_{p,m,l'} \gamma^{*}_{ml'}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}(\delta_{lm}\delta_{\uparrow\uparrow}\hat{b}^{\dagger}_{l'\uparrow} + \hat{b}^{\dagger}_{m\uparrow}\delta_{ll'}\delta_{\uparrow\uparrow})$$

For $l' = l$

$$[\hat{b}_{l\uparrow}, hc] = \sum_{p,m,l} \gamma^{*}_{ml}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}\hat{b}^{\dagger}_{m\uparrow} \tag{4.61}$$

Then, using Eq.(4.60) and Eq.(4.61) we get,

$$[\hat{b}_{l\uparrow}, \hat{H}_4] = \sum_{p,m,l} \gamma^{*}_{ml}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}\hat{b}^{\dagger}_{m\uparrow} \tag{4.62}$$

Substituting Eqs.(4.57), (4.60), (4.61) and (4.64) into Eq.(4.55) we get,

$$\omega << \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= 1 + << \epsilon_l \hat{b}_{l\uparrow} + U\hat{b}_{l\uparrow}\hat{b}^{\dagger}_{l\downarrow}\hat{b}_{l\downarrow} + \sum_{p,m,l} \gamma^{*}_{ml}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}\hat{b}^{\dagger}_{m\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>$$

$$= 1 + \epsilon_l << \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >> + U < \hat{b}^{\dagger}_{l\downarrow}\hat{b}_{l\downarrow} ><< \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>$$

$$+ << \sum_{p,m,l} \gamma^{*}_{ml} < \hat{a}_{p\uparrow}\hat{a}_{-p\downarrow} > \hat{b}^{\dagger}_{m\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>$$

$$(\omega - \epsilon_l - U < \hat{n}_{l\downarrow} >) << \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= 1 + \Delta^{*}_{l} << \hat{b}^{\dagger}_{m\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>$$

where, $\Delta^{*}_{l} = \sum_{p,m,l} \gamma^{*}_{ml} < \hat{a}_{p\uparrow}\hat{a}_{-p\downarrow} >$

$$<< \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= \frac{1 + \Delta^{*}_{l} << \hat{b}^{\dagger}_{m\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>}{\omega - (\epsilon_l + U < \hat{n}_{l\downarrow} >)} \tag{4.63}$$

we can also obtain the equation of motion for the exasperation $<< \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>$.

$$\omega << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>=< [\hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow}] > + << [\hat{b}^{\dagger}_{l'\uparrow}, \hat{H}], \hat{b}^{\dagger}_{l\uparrow} >>$$

$$\omega << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= 0 + << [\hat{b}^{\dagger}_{l'\uparrow}, \hat{H}], \hat{b}^{\dagger}_{l\uparrow} >> \tag{4.64}$$

The commutation can be calculated separately as follow.

$$[\hat{b}^{\dagger}_{l'\uparrow}, \hat{H}_1] = [\hat{b}^{\dagger}_{l'\uparrow}, \sum_{p,\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma} - \sum_{p,p'} V(pp')\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]$$

$$= \sum_{p,\sigma} \epsilon_p [\hat{b}^{\dagger}_{l'\uparrow}, \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}] - \sum_{p,p'} V(pp')[\hat{b}^{\dagger}_{l'\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{p'\downarrow}\hat{a}_{-p'\uparrow}]$$

$$[\hat{b}^{\dagger}_{l'\uparrow}, \hat{H}_1] = 0 \tag{4.65}$$

The commutation with $\hat{H}_2$ can be calculated as,

$$[\hat{b}^{\dagger}_{l'\uparrow}, \hat{H}_2] = [\hat{b}^{\dagger}_{l'\uparrow}, \sum_{m} \epsilon_m \hat{b}^{\dagger}_{m\sigma}\hat{b}_{m\sigma}] = \sum_{m} \epsilon_m [\hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{m\sigma}\hat{b}_{m\sigma}]$$

$$= \sum_{m} \epsilon_m ([\hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{m\sigma}]\hat{b}_{m\sigma} + \hat{b}^{\dagger}_{m\sigma}[\hat{b}^{\dagger}_{l'\uparrow}, \hat{b}_{m\sigma}])$$

$$= -\sum_{m} \epsilon_m \hat{b}^{\dagger}_{m\uparrow}\delta_{l'm}\delta_{\uparrow\uparrow}$$

Let, $m = l'$ and $\sigma = \uparrow$, then,

$$[\hat{b}^{\dagger}_{l'\uparrow}, \hat{H}_2] = -\epsilon_{l'}\hat{b}^{\dagger}_{l'\uparrow} \tag{4.66}$$

And, the commutation with the intra coulomb repulsion interaction Hamiltonian is also calculated as,

$$[\hat{b}^{\dagger}_{l'\uparrow}, \hat{H}_3] = [\hat{b}^{\dagger}_{l'\uparrow}, U\sum_{m} \hat{n}_{m\uparrow}\hat{n}_{m\downarrow}] = U\sum_{m} [\hat{b}^{\dagger}_{l'\uparrow}, \hat{n}_{m\uparrow}\hat{n}_{m\downarrow}]$$

$$= U \sum_m ([\hat{b}^\dagger_{l'\uparrow}, \hat{n}_{m\uparrow}]\hat{n}_{m\downarrow} + \hat{n}_{m\uparrow}[\hat{b}^\dagger_{l'\uparrow}, \hat{n}_{m\downarrow}])$$

$$= U \sum_m ([\hat{b}^\dagger_{l'\uparrow}, \hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}]\hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow} + \hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}[\hat{b}^\dagger_{l'\uparrow}, \hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow}])$$

$$= U \sum_m ([\hat{b}^\dagger_{l'\uparrow}, \hat{b}^\dagger_{m\uparrow}]\hat{b}_{m\uparrow}\hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow} + \hat{b}^\dagger_{m\uparrow}[\hat{b}^\dagger_{l'\uparrow}, \hat{b}_{m\uparrow}]\hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow} + \hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}[\hat{b}^\dagger_{l'\uparrow}, \hat{b}^\dagger_{m\downarrow}]\hat{b}_{m\downarrow}$$

$$+\hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}\hat{b}^\dagger_{m\downarrow}[\hat{b}^\dagger_{l'\uparrow}, \hat{b}_{m\downarrow}])$$

$$= -U \sum_m (\hat{b}^\dagger_{m\uparrow}\delta_{l'm}\delta_{\uparrow\uparrow}\hat{b}^\dagger_{m\downarrow}\hat{b}_{m\downarrow} + \hat{b}^\dagger_{m\uparrow}\hat{b}_{m\uparrow}\hat{b}^\dagger_{m\downarrow}\delta_{l'm}\delta_{\uparrow\downarrow})$$

For, $m = l'$

$$[\hat{b}^\dagger_{l'\uparrow}, \hat{H}_3] = -U\hat{b}^\dagger_{l'\uparrow}\hat{b}^\dagger_{l'\downarrow}\hat{b}_{l'\downarrow} \tag{4.67}$$

Similarly,

$$[\hat{b}^\dagger_{l'\uparrow}, \hat{H}_4] = [\hat{b}^\dagger_{l'\uparrow}, \sum_{p,m,l'} \gamma_{ml'}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{b}_{m\uparrow}\hat{b}_{l\uparrow} + hc]$$

$$[\hat{b}^\dagger_{l'\uparrow}, \hat{H}_4] = \sum_{p,m,l} \gamma_{ml}[\hat{b}^\dagger_{l'\uparrow}, \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{b}_{m\uparrow}\hat{b}_{l\uparrow}] + [\hat{b}^\dagger_{l'\uparrow}, hc] \tag{4.68}$$

$$\sum_{p,m,l} \gamma_{ml}[\hat{b}^\dagger_{l'\uparrow}, \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{b}_{m\uparrow}\hat{b}_{l\uparrow}] = \sum_{p,m,l} \gamma_{ml}([\hat{b}^\dagger_{l'\uparrow}, \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}]\hat{b}_{m\uparrow}\hat{b}_{l\uparrow} + \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}[\hat{b}^\dagger_{l'\uparrow}, \hat{b}_{m\uparrow}\hat{b}_{l\uparrow}])$$

$$= \sum_{p,m,l} \gamma_{ml}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}([\hat{b}^\dagger_{l'\uparrow}, \hat{b}_{m\uparrow}]\hat{b}_{l\uparrow} + \hat{b}_{m\uparrow}[\hat{b}^\dagger_{l'\uparrow}, \hat{b}_{l\uparrow}])$$

$$= \sum_{p,m,l} \gamma_{ml}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}(\delta_{l'm}\delta_{\uparrow\uparrow}\hat{b}_{l\uparrow} + \hat{b}_{m\uparrow}\delta_{l'l}\delta_{\uparrow\uparrow})$$

for, $m = l'$

$$\sum_{p,m,l} \gamma_{ml}[\hat{b}^\dagger_{l'\uparrow}, \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{b}_{m\uparrow}\hat{b}_{l\uparrow}] = \sum_{p,l} \gamma_{ml}\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{b}_{l\uparrow} \tag{4.69}$$

And,

$$[\hat{b}^\dagger_{l'\uparrow}, hc] = [\hat{b}^\dagger_{l'\uparrow}, \sum_{p,m,l} \gamma_{ml}\hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}\hat{b}^\dagger_{m\uparrow}\hat{b}^\dagger_{l'\uparrow}]$$

$$= \sum_{p,m,l} \gamma_{ml'}[\hat{b}^\dagger_{l'\uparrow}, \hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}\hat{b}^\dagger_{m\uparrow}\hat{b}^\dagger_{l'\uparrow}]$$

$$= \sum_{p,m,l} \gamma_{ml}([\hat{b}^\dagger_{l'\uparrow}, \hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}]\hat{b}^\dagger_{m\uparrow}\hat{b}^\dagger_{l'\uparrow} + \hat{a}_{p\uparrow}\hat{a}_{-p\downarrow}[\hat{b}^\dagger_{l'\uparrow}, \hat{b}^\dagger_{m\uparrow}\hat{b}^\dagger_{l'\uparrow}])$$

$$[\hat{b}^\dagger_{l'\uparrow}, hc] = 0 \tag{4.70}$$

Then, substituting Eqs.(4.69) (4.70) into Eq.(4.68) we get,

$$[\hat{b}^{\dagger}_{l'\uparrow}, \hat{H}_4] = \sum_{p,l} \gamma_{ml} \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} \hat{b}_{l\uparrow} \tag{4.71}$$

Now, substituting Eqs.(4.65), (4.66), (4.67) and (4.71) into Eq.(4.64) we get,

$$\omega << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>=<< -\epsilon_{l'} \hat{b}^{\dagger}_{l'\uparrow} - U \hat{b}^{\dagger}_{l'\uparrow} \hat{b}^{\dagger}_{l'\downarrow} \hat{b}_{l'\downarrow} + \sum_{p,l} \gamma_{ml} \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>$$

$$\begin{aligned} \omega << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= -\epsilon_{l'} << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >> -U < \hat{n}_{l'\downarrow} ><< \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >> \\ + \sum_{p,l} \gamma_{ml} < \hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} ><< \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >> \\ = -\epsilon_{l'} << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >> -U < \hat{n}_{l'\downarrow} ><< \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >> + \Delta_l << \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >> \\ (\omega + \epsilon_{l'} + U < \hat{n}_{l'\downarrow} >) << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= \Delta_l << \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >> \end{aligned}$$

$$<< \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= \frac{\Delta_l << \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>}{\omega + (\epsilon_{l'} + U < \hat{n}_{l'\downarrow} >)} \tag{4.72}$$

But, from Eq.(4.63) we have,

$$<< \hat{b}_{l\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= \frac{1 + \Delta^*_l << \hat{b}^{\dagger}_{m\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>}{\omega - (\epsilon_{l'} + U < \hat{n}_{l\downarrow} >)}$$

$$<< \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= \frac{\Delta_l}{\omega + (\epsilon_{l'} + U < \hat{n}_{l\downarrow} >)} \frac{(1 + \Delta_l << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>)}{\omega - (\epsilon_{l'} + U < \hat{n}_{l\downarrow} >)}$$

where $m = l'$, $\hat{n}_{l'\downarrow} = \hat{n}_{l\downarrow}$ and $\Delta^*_l = \Delta_l$

$$(\omega^2 - (\epsilon_{l'} + U < \hat{n}_{l\downarrow} >)^2) << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= \Delta_l + \Delta^2_l << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>$$

Solving for $<< \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>$ we get,

$$<< \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >>= \frac{\Delta_l}{\omega^2 - (\epsilon_{l'} + U < \hat{n}_{l\downarrow} >)^2 - \Delta^2_l} \tag{4.73}$$

4.2.3 Equation of Motion That Shows The Correlation Between Conduction and Localized Electrons

The equation of motion that shows the correlation between the conduction and localized electrons is given below. Using similar definition as for Δ, we can write the parameter η as,

$$\eta = \frac{\alpha}{\beta} \sum_{k,n} << \hat{b}^{\dagger}_{l'\uparrow}, \hat{b}^{\dagger}_{l\uparrow} >> \tag{4.74}$$

Using Eq.(4.73) into Eq.(4.74) we have,

$$\eta = \frac{\alpha}{\beta}\sum_{k,n}\frac{\Delta_l}{\omega^2 - (\epsilon_{l'} + U < \hat{n}_{l\downarrow} >)^2 - \Delta_l^2}$$

$$\eta = \frac{\alpha}{\beta}\sum_{k,n}\frac{\Delta_l}{w^2 - \epsilon_l^2 - \Delta_l^2}$$

where, $\epsilon_{l'} + U < \hat{n}_{l\downarrow} >= \epsilon_l$
Changing the summation into integration by introducing the density of state $N(0)$ at the Fermi level, $\sum_k \rightarrow \int_{-\epsilon_f}^{\infty} d\epsilon N(0)$, we obtain,

$$\eta = \frac{\alpha}{\beta}\sum_{n}\int_{-\epsilon_f}^{\infty} d\epsilon N(0)\frac{\Delta_l}{\omega^2 - \epsilon_l^2 - \Delta_l^2}$$

$$\eta = \frac{-2\alpha}{\beta}N(0)\sum_{n}\int_{0}^{\hbar\omega_b} d\epsilon\frac{\Delta_l}{\omega_n^2 + \epsilon_l^2 + \Delta_l^2} \quad (4.75)$$

Using $\omega = i\omega_n$ and the Matsubara frequency $\omega_n = (2n+1)\frac{\pi}{\beta}$ Eq.(4.75) becomes,

$$\eta = -2N(0)\alpha\beta\sum_{n}\int_{0}^{\hbar\omega_b} d\epsilon\frac{\Delta_l}{(2n+1)^2\pi^2 + E^2\beta^2} \quad (4.76)$$

where, $E^2 = \epsilon_l^2 + \Delta_l^2$ Using the relation $\frac{1}{2x}tanh(\frac{x}{2}) = \sum_n \frac{1}{(2n+1)^2\pi^2+x^2}$, Eq.(4.76) becomes,

$$\eta = -2\alpha\beta N(0)\int_{0}^{\hbar\omega_b} d\epsilon\frac{\Delta_l}{2(\beta E)}\tanh(\frac{\beta E}{2}) \quad (4.77)$$

Let, $N(0)\alpha = \lambda_l$, then Eq.(4.77) becomes,

$$\eta = -\lambda_l\Delta_l\int_{0}^{\hbar\omega_b} d\epsilon\frac{1}{\sqrt{\epsilon_l^2 + \Delta_l^2}}\tanh(\frac{\beta\sqrt{\epsilon_l^2 + \Delta_l^2}}{2}) \quad (4.78)$$

One can also write Eq.(4.78) as,

$$\eta = -\lambda_l\Delta_l\int_{0}^{\hbar\omega_b}\frac{2}{\beta}\sum_{n=-\infty}^{\infty}\frac{d\epsilon}{\omega_n^2 + \epsilon_l^2 + \Delta_l^2} \quad (4.79)$$

Using the Laplace transformation and Matsubara frequency $\omega_n = (2n+1)\frac{\pi}{\beta}$, Eq.(4.79) becomes,

$$\frac{-\eta}{\lambda_l\Delta_l} = \int_{0}^{\hbar\omega_b}\frac{2}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{\omega_n^2 + E^2}dE - \int_{0}^{\hbar\omega_b}\Delta_l^2\frac{2}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{(\omega_n^2 + E^2)^2}dE + ... \quad (4.80)$$

$$= \int_{0}^{\hbar\omega_b}\frac{1}{E}\tanh(\frac{\beta E}{2})dE - \int_{0}^{\hbar\omega_b}\Delta_l^2\frac{2}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{(((2n+1)\frac{\pi}{\beta})^2 + E^2)^2}dE$$

Let, $a^2 = ((2n+1)\frac{\pi}{\beta})^2$

$$\frac{-\eta}{\lambda_l \Delta_l} = \int_0^{\hbar\omega_b} \frac{1}{E}\tanh(\frac{\beta E}{2})dE - \int_0^{\hbar\omega_b} \Delta_l^2 \frac{2}{\beta} 2 \sum_0^{\infty} \frac{dE}{a^4(1+x^2)^2} + ... \tag{4.81}$$

where, $x^2 = \frac{E^2}{a^2}$

$$\frac{-\eta}{\lambda_l \Delta_l} = I_1 + I_2$$

$$I_1 = \int_0^{\hbar\omega_b} \frac{1}{E}\tanh(\frac{\beta E}{2})dE$$

Let, $y = \frac{\beta E}{2}$, then, $dy = \frac{\beta}{2}dE$

$$I_1 = \int_0^{y} \frac{1}{y} tanh(y) dy$$

$$= \ln(y)\tanh(y)|_0^y - \int_0^y \frac{\ln(y)}{\cosh^2(y)}dy \tag{4.82}$$

Fo low temperatures ($T \to 0K$ or $T \to T_m$), $\tanh(\frac{E}{2k_BT}) \to 1$. Thus, we get,

$$I_1 = ln(\frac{E}{2k_BT_m}) - ln(\frac{\pi}{4\gamma}) \tag{4.83}$$

where, γ is the Euler constant having the value $\gamma = 1.78$

$$I_1 = \ln 1.14 \frac{\hbar w_b}{k_B T_m} \tag{4.84}$$

And

$$I_2 = -\int_0^{\hbar\omega_b} \Delta_l^2 \frac{2}{\beta} 2 \sum_0^{\infty} \frac{dE}{a^4(1+x^2)^2} + ...$$

$$= -\frac{4\Delta_l^2}{\beta} \int_0^{\hbar\omega_b} \sum_0^{\infty} \frac{adx}{a^4(1+x^2)^2} + ...$$

$$= -4\Delta_l^2 \sum_0^{\infty} \frac{\beta^2}{(\pi(2n+1))^3} \int_0^{\infty} \frac{1}{(1+x^2)^2}dx + ...$$

$$= \frac{-4\beta^2}{\pi^3}\Delta_l^2 \frac{7}{8}\zeta(3)\frac{\pi}{4}$$

$$I_2 = -(\frac{\Delta_l}{\pi k_B T_m})^2 (\frac{8.414}{8}) \tag{4.85}$$

where, $\int_0^{\infty} \frac{1}{(1+x^2)^2}dx = \frac{\pi}{4}$ and $\sum_{n=0}^{\infty}(\frac{1}{(2n+1)^P} = (1-2^{-p})\zeta(p)$, $p = 3$, $\zeta(3) = 1.202$, ζ is zeta function.

Then, substituting Eqs.(4.84), (4.85) into Eq.(4.80), we get,

$$\eta \approx -\lambda_l \Delta_l (ln(1.14\frac{\hbar w_b}{k_B T_m}) - \Delta_l^2 (\frac{1}{\pi k_B T_m})^2 (\frac{8.414}{8}))$$

$$\eta \approx -\lambda_l\Delta_l ln(1.14\frac{\hbar\omega_b}{k_BT_m}) + \lambda_l\Delta_l^3(\frac{1}{\pi k_BT_m})^2(\frac{8.414}{8}) \tag{4.86}$$

Since Δ_l is very small, Δ_l^3 can be neglected Eq.(4.86) becomes,

$$\eta \approx -\lambda_l\Delta_l ln(1.14\frac{\hbar\omega_b}{k_BT_m})$$

Solving for T_m, we get,

$$T_m = 1.14\frac{\hbar\omega_b}{k_B}\exp(\frac{\eta}{\lambda_l\Delta_l}) \tag{4.87}$$

4.3 For Pure Superconducting System

For pure superconducting system, that is, when magnetic effect is zero, we can ignore the η term and our previous calculation yield a result which is in agreement with the well-established BCS model as shown below.

Using Eq.(4.34), as, $T \to 0$, $\eta \to 0$ and $\tanh(\frac{\beta\epsilon}{2}) \to 1$, it reduces to,

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega_b} \frac{\Delta}{\sqrt{\epsilon_k^2 + \Delta^2}} d\epsilon_k$$

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} \frac{1}{\sqrt{\epsilon_k^2 + \Delta^2}} d\epsilon_k = \sinh^{-1}(\frac{\hbar\omega_b}{\Delta})$$

which implies,

$$\sinh(\frac{1}{\lambda}) = \frac{\hbar\omega_b}{\Delta}$$

$$\frac{e^{\frac{1}{\lambda}} - e^{\frac{-1}{\lambda}}}{2} = \frac{\hbar\omega_b}{\Delta}$$

Since, $e^{\frac{-1}{\lambda}}$ is small, we can ignoring it, and solving for Δ, we get,

$$\Delta(0) = 2\hbar\omega_b \exp(\frac{-1}{\lambda}) \tag{4.88}$$

As $T \to T_c$, for $\eta = 0$,

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} \frac{tanh(\frac{(\beta\epsilon_k)}{2})}{\epsilon_k} d\epsilon_k$$

$$= \int_0^{\frac{\beta}{2}\hbar\omega_b} \frac{tanh(y)}{y} dy$$

where, $y = \frac{\beta\epsilon_k}{2}$

$$\frac{1}{\lambda} = ln(y)\tanh(y)|_0^{\frac{\beta}{2}\hbar\omega_b} - \int_0^{\frac{\beta}{2}\hbar\omega_b} \frac{ln(y)}{cosh^2(y)} dy$$

For low temperature, $tanh(\frac{\hbar\omega_b}{2k_BT}) \to 1$

$$\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_BT_c})$$

$$k_BT_c = 1.14\hbar w_b \exp{(-\frac{1}{\lambda})} \tag{4.89}$$

In order to obtain temperature dependence of energy gap of Eq.(4.34), we follow the same technique to solve the following integral.

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} d\epsilon \frac{1}{\sqrt{\epsilon^2+\Delta^2}} tanh(\frac{\beta\sqrt{\epsilon^2+\Delta^2}}{2})$$

$$= ln(1.14\frac{\hbar\omega_b}{k_BT}) - \Delta^2(\frac{1}{\pi k_BT})^2\frac{8.414}{8} + ... \tag{4.90}$$

But from the BCS model, at, $T = T_c$, $\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_BT_c})$, and $\omega_b = \omega_D$, from this we obtain,

$$ln(\frac{T}{T_c}) = -\Delta^2(\frac{1}{\pi k_BT_c})^2(\frac{8.414}{8}) + ... \tag{4.91}$$

Using, $ln(1-x) = -x - \frac{(1-x)^2}{2} + ...$, we get,

$$ln(\frac{T}{T_c}) = (1 - (1 - \frac{T}{T_c}))$$

$$= -(1 - \frac{T}{T_c}) - \frac{(1-\frac{T}{T_c})^2}{2} + ...$$

$$ln(\frac{T}{T_c}) \approx -(1 - \frac{T}{T_c})$$

$$-(1 - \frac{T}{T_c}) \approx -\Delta^2(\frac{1}{\pi k_BT_c})^2(\frac{8.414}{8})$$

$$\Delta(T) = 3.06k_BT_c(1 - \frac{T}{T_c})^{\frac{1}{2}} \tag{4.92}$$

This is the expression that shows how the superconducting order parameter (Δ) varies with temperature when the magnetic order parameter (η) is zero and is similar to the BCS model.

CHAPTER 5

Results and Discussion

In this part of our study, we have discussed the results which are obtained in chapter four using the model Hamiltonian developed. We obtained the expressions for the superconducting order parameter (Δ) and magnetic order parameter (η) with respect to superconducting transition temperature (T_c) and magnetic order temperature (T_m) respectively. The superconducting order parameter (Δ) is expressed as a function of temperature (T) in Eq(4.92) and is plotted in Fig.(5.1). It shows the superconducting order parameter, which is the measure of pairing energy decreases with increasing temperature and vanishes at a critical temperature $T_c = 8K$ for the superconductor $CeO_{1-x}F_xBiS_2$. For pure superconductor, i.e when the magnetic order parameter ($\eta = 0$), the expression we obtain in Eq.(4.92) is in a good agreement with the BCS model.

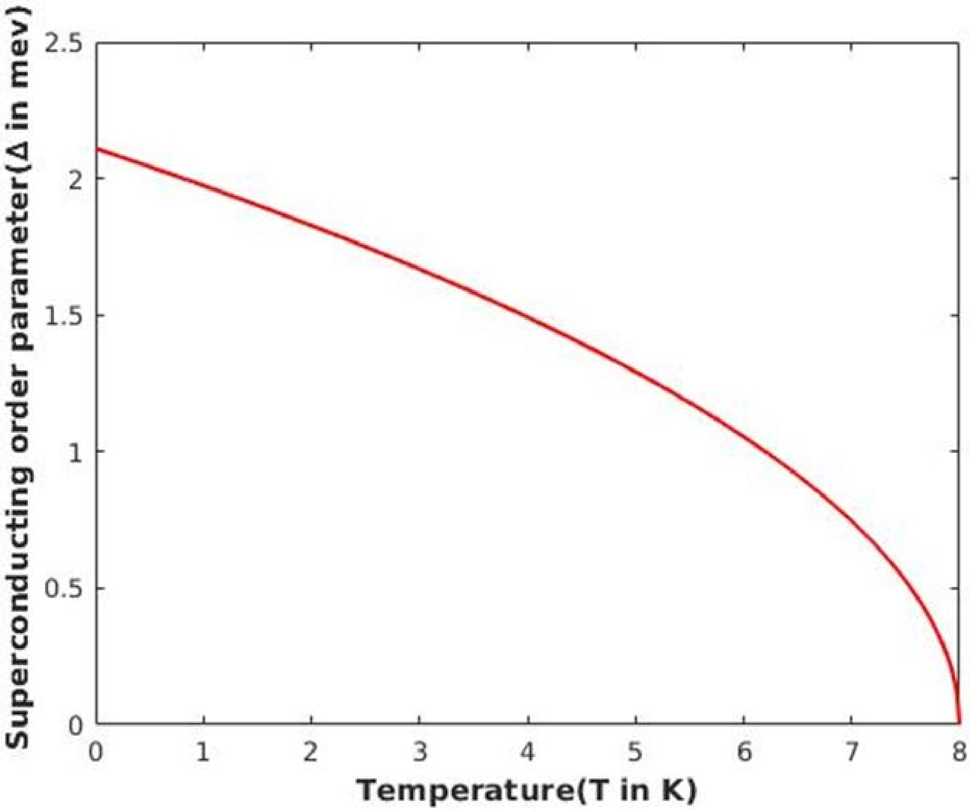

Figure 5.1: Superconducting order parameter versus Temperature for superconductor $CeO_{1-x}F_xBiS_2$ at x=0.7.

Furthermore, the transition temperature (T_c) has been evaluated numerically as a function of magnetic order parameter (η). Using the experimental value of T_c for the superconductor $CeO_{1-x}F_xBiS_2$ and some plausible approximations for other parameters, we plotted the transition temperature (T_c) versus magnetic order parameter (η) as shown in Fig.(5.2).

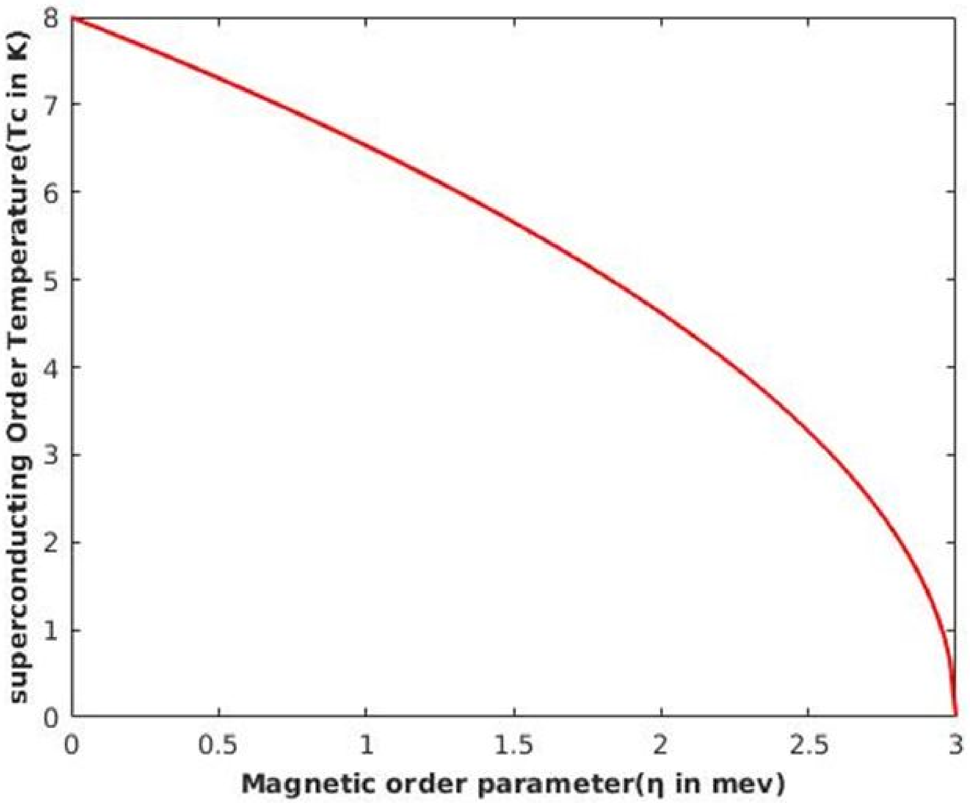

Figure 5.2: Superconducting transition temperature versus magnetic order parameter for the superconductor $CeO_{1-x}F_xBiS_2$ at x=0.7.

Fig.(5.2) shows that, when the magnetic ordering parameter increases the superconducting transition temperature decreases. For this purpose, we have used Eq.(4.39).

By employing Eq.(4.87), and using the experimental value, $T_m = 7.5K$ for the superconductor $CeO_{1-x}F_xBiS_2$ and some suitable approximations for the other parameters in the equation, we plotted the magnetic order temperature versus magnetic order parameter as demonstrated in Fig.(5.3). From the figure we can observe that, as the magnetic order parameter increases the magnetic order temperature also increases.

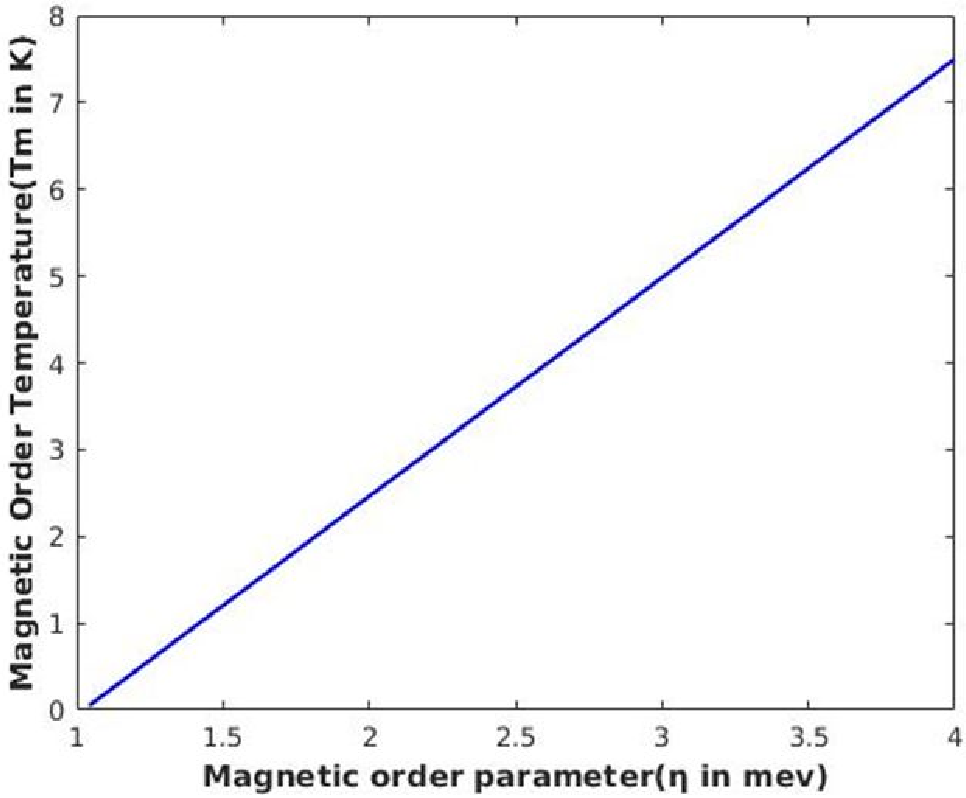

Figure 5.3: Magnetic transition temperature versus magnetic order parameter for the superconductor $CeO_{1-x}F_xBiS_2$ at x=0.7.

Now, by merging Figs.(5.2) and (5.3), we get a region in which both superconductivity and ferromagnetism coexists as shown in Fig.(5.4). Thus, our finding is in agreement with the experimental findings [18].

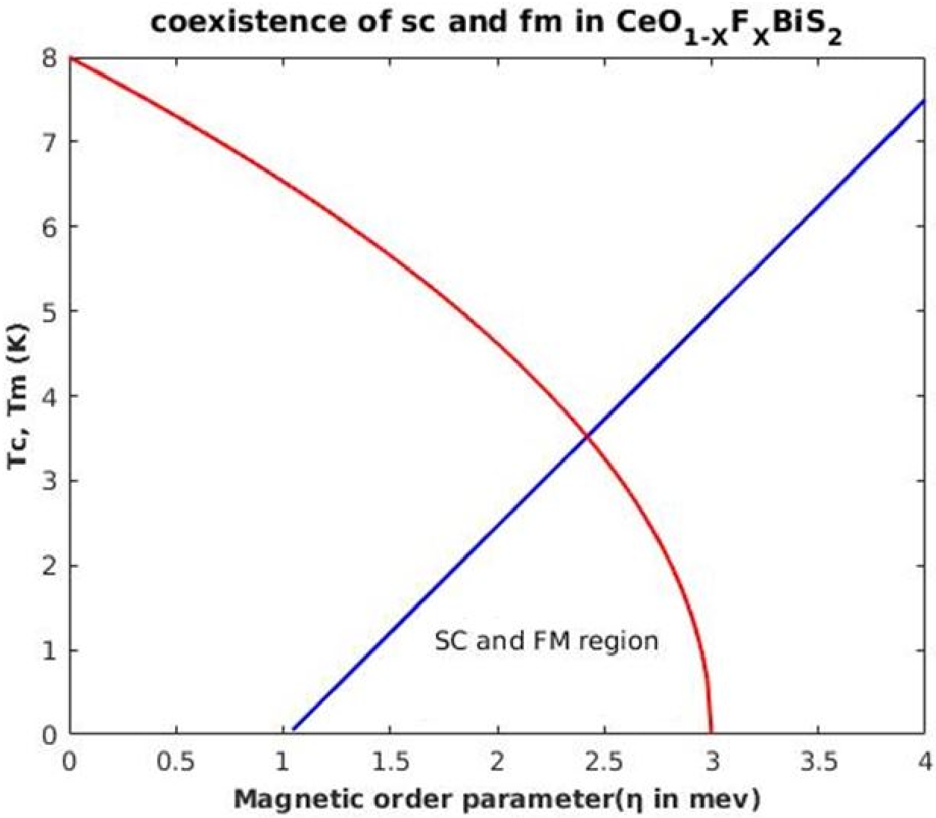

Figure 5.4: Superconducting temperature and magnetic ordering temperature versus magnetic order parameter for the superconductor $CeO_{1-x}F_xBiS_2$ at x=0.7.

In this study, Eq.(4.78) shows the correlation of the mobile and the localized electrons, and since η, corresponds to the localized electrons, we see that the two parameters are related to each other. This shows the contribution of both the mobile and the localized electrons and hence the combined phenomenon of superconductivity and ferromagnetism is manifested.

CHAPTER 6

Conclusion

In the present work, we have demonstrated the basic concepts of superconductivity with special emphasis on the BCS model pairing focused on the interaction between superconductivity and ferromagnetism which are closely connected to superconductor $CeO_{1-x}F_xBiS_2$. By employing the double time temperature dependent Green's function formalism, we developed the model Hamiltonian for the system and derived equations of motion for conduction electrons, localized electrons and for pure superconducting system and carried out various correlations by using suitable decoupling procedures. In developing the model Hamiltonian, we considered spin triplet pairing mechanism and obtained expressions for superconducting order parameter, magnetic order parameter, superconducting transition temperature and magnetic order temperature. By using appropriate experimental values and considering suitable approximations, we plotted phase diagrams using the equations we developed. As is well-known, superconductivity and ferromagnetism are two cooperative phenomena which are mutually antagonistic since superconductivity is associated with the pairing of electron states related to time reversal while in the magnetic states the time reversal symmetry is lost. Because of this, there is a strong competition between the two phases. This competition between superconductivity and magnetism made coexistence unlikely to occur. However, as can be seen from Fig.(5.4), we have observed that, there is a wide region that shows, the coexistence of ferromagnetism and bulk superconductivity in superconductor $CeO_{1-x}F_xBiS_2$ annealed under high pressure. Furthermore, the plotted phase diagrams suggest that superconductivity in the BiS_2 layers and ferromagnetism in the CeO layers are linked to each other.

References

[1] H. Kamerlingh Onnes, Akad. Weten Schappen (Amsterdam) **14**, 113(1911).

[2] Griffin, Allan. "New light on the intriguing history of super fluidity in liquid ^4He." Journal of Physics: Condensed Matter **21**, 164220(2009).

[3] S. Lange and C. Timm theory of superconductivity Institute of Theoretical Physics Tu Dresden Version 6 (2012), Germany

[4] Christian Barth, High Temperature Superconductor Cable Concepts for Fusion Magnets, KIT scientific publishing, ISSN: **74**, 1869(2013)

[5] Hammad, Ibrahim Adam Ibrahim, et al. "Pressure Effect on Superconducting Critical Temperature According to String Model." International Journal of Fluid Mechanics Thermal Sciences **3**, 70(2017).

[6] Eiji Muromachi,now international **7** ,4(2009).

[7] W. Meissner and R. Ochsenfeld, Naturwiss **21**, 787(1933).

[8] Matthias, Bernd T. "magnetization curves of superconductors-type I and type II." Proceedings of the 1972 Proton Linear Accelerator Conference, October 10, 1972. US Atomic Energy Commission, Technical Service Center,**1**, 13(1972).

[9] Webb, G. W., F. Marsiglio, and J. E. Hirsch. "Superconductivity in the elements, alloys and simple compounds." Physica C: Superconductivity and its applications **17**, 514(2015).

[10] Bardeen, John, Leon N. Cooper, and John Robert Schrieffer. "Theory of superconductivity." Phys Rev. **108**, 1175(1957).

[11] Mizuguchi, Yoshikazu. "Review of superconductivity in BiS_2-based layered materials." Journal of Physics and Chemistry of Solids **84**, 34(2015).

[12] Y. Kamihara, T. Watanabe, M. Hirano, H. Hobson, J. Am. Chem. Soc. **130**, 3296(2008).

[13] Y. Mizuguchi, H. Fujihisa, Y. Gotoh, K. Suzuki, H. Usui, K. Kuroki, S. Demura, Y. Takano, H. Izawa, O. Miura, Phys. Rev. B **86**, 220510(2012).

[14] Wakita, Takanori, et al. "Ce 4f electronic states of $CeO_{1-x}F_xBiS_2$ studied by soft x-ray photoemission spectroscopy." Physical Review B **95**, 085109(2017).

[15] Paris, E, et al. "Determination of local atomic displacements in $CeO_{1-x}F_xBiS_2$ system." Journal of Physics: Condensed Matter **26**, 435701 (2014).

[16] Abuladze, Grigol. Interplay Between Magnetic and Superconducting Layers in Thin Film Heterostructure. Diss. Georgian Technical University, **5**, 52425(2016).

[17] Jiles, David. Introduction to magnetism and magnetic materials. CRC press **13**, 01001(2014).

[18] Demura, Satoshi, et al. "Coexistence of Bulk Superconductivity and Magnetism in $CeO_{1-x}F_xBiS_2$." Journal of the Physical Society of Japan **84**, 024709(2015).

[19] Felner, I. "Coexistence of Superconductivity and Magnetism in $R_{2-x}ce_xRuSr_2Cu_2O_{10-d}$ (R=Eu and Gd)." arXiv preprint cond-mat **8**, 0211533(2002).

[20] Ginsburg, V.L. Ferromagnetic Superconductors. Soviet Physics,JETP, **4**, 153(1957).

[21] Matthias, B.T., Suhl, H. and Corenzwit, E. Spin Exchange in Superconductors. Phys.Rev.Let, **1**, 92(1958).

[22] Brhane, Haftu. "Coexistence of Superconductivity and Ferromagnetism in Intermetallic Uranium-Based Superconductors UCoGe, UIr and UGe_2." **4**, 2250(2014).

[23] Aoki, D., Huxley, A., Ressouche, E., Braithwaite, D., Flouquet, J., Brison, J.P., Lhotse, E. and Paulsen, C. Coexistence of Superconductivity and Ferromagnetism in URhGe. Nature, **413**, 613(2001).

[24] Pfleiderer, C., Uhlarz, M., Hayden, S.M., Vollmer, R., Lohneysen, H.V., Bernhoeft, N.R. and Lonzarich, G.G. Coexistence of Superconductivity and Ferromagnetism in the d-Band Metal $ZrZn_2$. Nature, **412**, 58(2001).

[25] Saxena, S.S., Agarwal, P., Ahilan, K., Grosche, F.M., Haselwimmer, R.K.W., Steiner, M.J., Pugh, E., Walker, I.R., Julian, S.R., Monthoux, P., Lonzarich, G.G., Huxley, A., Sheikin, I., Braithwaite, D. and Flouquet, J. Superconductivity on the Border of Itinerant-Electron Ferromagnetism in UGe_2 Superconductivity. Nature, **406**, 587(2000).

[26] Singh, P. "Coexistence of Superconductivity and Ferromagnetism." Journal of superconductivity and Novel magnetism **24**, 945(2011).

[27] D.v.Shopova,T.E.Tsuetkov,D.I.U Zunov,Condensd matter Physics, **8**, 41(2005).

[28] N. T. Huy, A. Gasparini, D. E. de Nijs, Y. Huang, J. C. P. Klaasse, T. Gortenmulder, A. de V isser; A. Hamann, T. Gorlach, and H. v. Lohneysen, Physical Review letters (PRL) **99**, 067006(2007).

[29] Sugimoto, T., et al. "Metallic phase in stoichiometric $CeOBiS_2$ revealed by space-resolved ARPES." Scientific reports **8**, 41598(2018).

[30] Sugimoto, Takuya, et al. "Anderson's impurity-model analysis on $CeO_{1-x}F_xBiS_2$." Journal of Physics: Conference Series. **592**, 012073(2015).

[31] J. Xing, S. Li, X. Ding, H. Yang, H.H. Wen, Phys. Rev. B **86**, 214518(2012).

[32] Kajitani, Joe, et al. "Increase in Tc and Change of Crystal Structure by High-Pressure Annealing in BiS_2-Based Superconductor $CeO_{0.3}F_{0.7}BiS_2$." Journal of Superconductivity and Novel Magnetism **28**, 1129(2015).

[33] H. Usui, K.Suzuki, K.Kuroki, Phys. Rev. B **86**, 220501(2012).

[34] Kuzemsky, A. L. "Irreducible Green functions method and many-particle interacting systems on a lattice." arXiv preprint cond-mat **25**, 0208219(2002).

[35] A.J. Legget, Rev. Mod. Phys. **47**, 331(1975).

Declaration

I hereby declare that this thesis is my original work and has not been presented for a degree in any other university. All sources of material used for the thesis have been duly acknowledged.

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