THE STUDY ON SUPERCONDUCTIVITY OF LIFEAS DUE TO INCIPIENT BAND

By

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Abstract

To study the superconductivity of LiF eAs due to incipient band the suitable Hamiltonian was formulated using the free and localized electrons, the electron-electron interaction through fermion exchange and the interaction term between free electro and localized electron due to incipient band. The formulation of Hamiltonian was invited us to derive the EOM for the entire system. Using the EOM we have theoretically calculated both the superconducting energy gap $\Delta(0)$ and transition temperature T_c which are including magnetic order parameter ϑ. As we are concerning a pure superconductor to approximate $\Delta(0)$ and T_c, the McMillan's formula has been adopted. As a result we have theoretically calculated the value of critical temperature to be 17.37K and the superconducting energy gap to be 4.5mev. Theoretically calculated values were come into comparison with the experimental value and finally we conclude that in a well established system electron pairing due to incipient band can possibly enhance superconductivity of materials.

keywords: Superconductivity, incipient band,T_c

Chapter 1

Introduction

1.1 Background of The Study

The beginning of the twentieth century saw a revolution in theoretical physics. The new physics, and in particular quantum mechanics, met with success after success, it explained the ultraviolet catastrophe, the photoelectric effect, the Compton effect, the structure of the atom and even made the prediction of antimatter[1-2]. This advance on all fronts has been challenged by the two phenomena of super fluidity of helium and superconductivity of metals. The emerging of superconductivity had date back 100 years. It was in 1908 where the Dutch physicist H.Kamerlingh Onnes initiated the field of low-temperature physics by liquefying helium in his laboratory at Leiden. Three years later he investigated that below 4.15K of the DC resistance of mercury dropped to zero [3]. With that investigation the concept of superconductivity was born.

Experimentalists were intended to search more knowledge on the superconductivity after the declaration of the existence of new physics (superconductivity). Accordingly, in 1933, Meissner and Ochsenfeld approved that; when a specimen is placed in a magnetic field and is then cooled below transition temperature for superconductivity, the magnetic flux originally present is ejected from the specimen [1-3]. This time a superconductor which is weak in magnetic field will act as a perfect diamagnetic. Then, in the 1950s and 1960s, a remarkably complete and satisfactory theoretical picture of the classic superconductors(including London equation and Ginsburg Landau theory) was emerged [3]. As all previous (low-temperature) superconductors require expensive liquid helium to cool them to around 4K[21]. Also, substantial skill and training is required to transfer liquid helium from one container to another without freezing the apparatus and the superconductors were rarely used in applications. Moreover the cost of the superconductor will always be substantially higher than that of a conventional conductor, it must bring overwhelming cost effectiveness to the system[25]. This situation was overturned and the subject was revitalized in 1986, when the new class of high-temperature superconductors was discovered by Bednorz and Müller, which was paving the way for a gradual proliferation of superconductivity and it was time at which people believed that superconductivity is a "mature" physics. Following this, for the first time the very important category of compound known as FeSC was observed in 2008 by Hideo Hosono (from the Tokyo Institute of Technology in Japan) in LaOFFeAs (1111 family)[18,55].

These FeSCs are divided into six different structure of FeAs layer families and out of these the '111' family consists LiF eAs which is under investigation of our work. This compound has been studied experimentally and theoretically whose T_c value reaches 18K[44]. As LiF eAs is apparently a key compound for the mechanism of superconducting in FeSCs, and it is a very remarkable member in the family of '111' we are interested to study the superconductivity of LiF eAs due to incipient band.

1.2 Statement of the problem

Recent experiments on certain FeSCs hinted at a role for paired electrons in "incipient" bands that are close to, but do not cross the Fermi level [14]. On the other hand theoretical works disagree on whether or not strong-coupling superconductivity is required to explain such effects, and whether critical interaction strength exists. Getting high temperature superconductor is the current issue, because of cooling materials so expensive[24]. There are different mechanisms of increasing T_c by extending the original BCS theory. Thus; this study would like to emphasize, the theoretical analysis on the superconductivity of LiFeAs due to incipient band.

1.3 Objectives of the Study

General Objective

The general objective of the study is to investigate the theoretical analysis on superconductivity of LiFeAs due to incipient band.

Specific Objectives

The specific objectives of the study are:

- To model a suitable Hamiltonian that can capture the contribution of incipient band.
- To calculate the superconducting energy gap of LiF eAs at low temperature (T=0K).
- To calculate the superconducting transition temperature T_c of LiF eAs due to incipient band.

Chapter 2

Review of Literature

2.1 Existence of Superconductivity

Superconductivity is widely regarded as one of the great scientific discoveries of the 20th Century[25]. This miraculous property causes certain materials, at low temperatures, to lose all resistance to the flow of electricity[24]. This state of ”losslessness” enables a range of innovative technology applications. The era of low-temperature physics began in 1908 when the Dutch physicist Kamerlingh Onnes first liquefied helium, which boils at 4.2K at standard pressure. Three years later, in 1911, in the Leiden laboratory of Kamerlingh Onnes and one of his assistants discovered the phenomenon of superconductivity while studying the resistivity of metals at low temperature. At that time it was noticed that the resistivity of Hg metal vanished suddenly at about 4.2K[1].

The macroscopic quantum phenomenon at which the electrical resistivity of many metals and alloys drops suddenly to zero at particular temperature called critical temperature Tc is known to be superconductivity[2]. At a critical temperature T_c, the specimen undergoes a phase transition from a state of normal electrical resistivity to a superconducting state. Below T_c resistivity is zero, not just close to zero. In Figure 2.1 it was shown that the historical electrical measurement of superconductivity in mercury in 1911. According to Onnes, Mercury has passed into a new state, which on account of its extraordinary electrical properties which is called the super-conductive state[1-2].

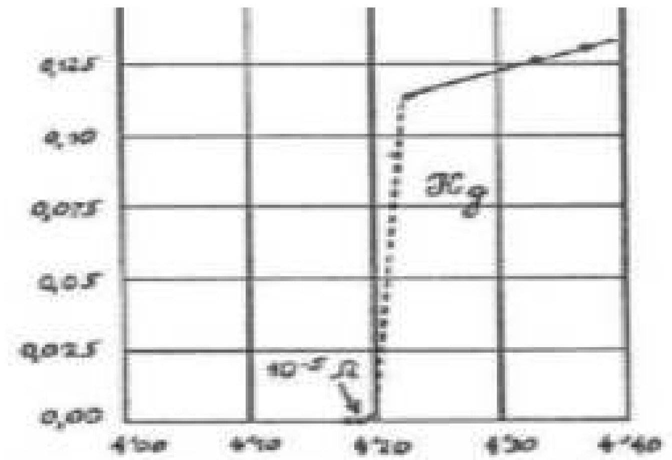

Figure 2.1: The critical temperature of Hg drops to 4.2K and it becomes superconductor below this temperature as discovered by Kamerlingh Onnes in 1911[1].

After this discovery a number of superconductors involving elements alloys, and compounds were invented at different critical temperature such that some of them are listed below[1,10,13].

Materials	Ti	Al	Hg	Sn	Pb	Nb	Nb_3Sn	NbGE	Mg_2	$YB_2Cu_3O_6$
T_c(K)	0.4	1.14	4.15	3.72	7.9	9.2	18	23.2	39.0	90.0

There are two most striking features of a superconducting materials[5,10,13]:

1. Perfect conductivity: zero resistance (no power loses).

2. Perfect diamagnetism: very strong repulsion in magnetic fields.

Superconductivity of a material can be destroyed by application of sufficiently large magnetic field as well as if the current exceeds a critical current[1,3,10]. The magnetic field above which the superconductor becomes normal state is critical field Hc. This critical field is related thermodynamically to the free energy difference between the normal and superconducting states in zero field, the so called condensation energy of superconducting state[3], which is more precisely named as thermodynamic critical field(H_c). It can be determined by equating the energy ($\frac{H^2}{8\pi}$) per unit volume, associated with holding the field out against the magnetic pressure with the condensation energy as follow:

$$\frac{H_c^2}{8\pi} = f_n(T) - f_s(T) \tag{2.1}$$

Where f_n and f_s are the Helmholtz free energy per unit volume in the respective phases of zero field and $H_c(T)$ is found empirically through approximation by a parabolic law[3].

$$H_c(T) \approx H_c(0)[1 - (\frac{T}{T_c})^2] \tag{2.2}$$

A discovery of enormous practical consequences was finding that there exist two types of superconductors with rather different response to Ginsberg Landau parameter and magnetic fields which will discussed in sections 2.6 and 2.7 respectively.

2.2 Meissner Effect

One of the properties of superconducting material is expelling magnetic fields from its interior by generating electrical currents on the surface which is known as the Meissner effect[24]. It is very suggestive that the process of expulsion of magnetic field and transition to the superconducting state of a macroscopic sample occurs through radial expansion of small superconducting regions[11]. It was discovered in 1933 without any theoretical basis, by W. Meissner and R.Ochsnfield [3,8]. This happens due to the screening currents, which are currents that the superconductor makes with its super currents, to screen out any magnetic fields attempting to penetrate the material. That is what causes the materials to expel the magnetic field[13]. When a superconductor below T_c is placed under weak external magnetic field B, it repels the magnetic flux(field)B completely from its interior[8]. By expelling the field and thus distorting nearby magnetic field lines, as shown in Figure 2.2, a superconductor will create a strong enough force field to overcome gravity[21]. Superconductors in the Meissner state exhibit perfect diamagnetism, which means that the total magnetic field is close to zero deep inside the superconductor[2]. By Lenz's law a current generated, which opposes the flux and cancel out any magnetic field from the superconductor[8,11,13].

The repulsion occurs only if the strength of the applied magnetic field does

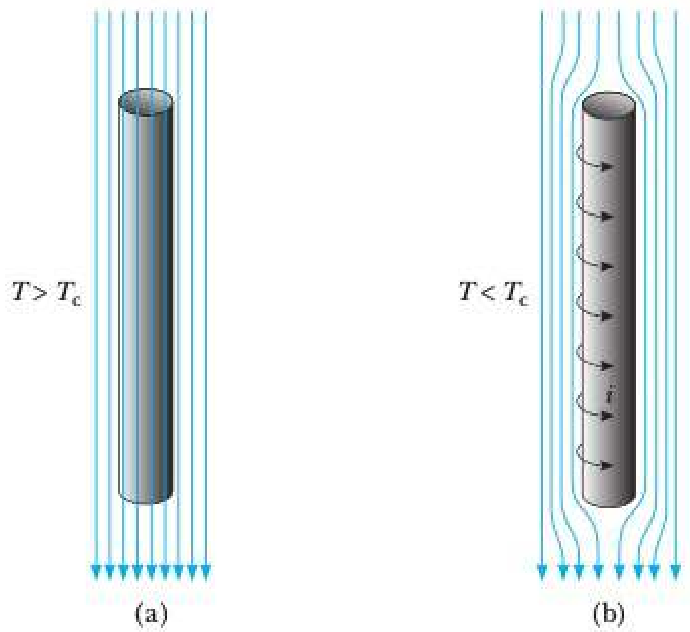

Figure 2.2: A superconductor in the form of a long cylinder in the presence of an external magnetic field. (a) At temperature above T_c, the field lines penetrate the cylinder because it is in its normal state. (b) When the cylinder is cooled to $T < T_c$ and becomes superconducting, magnetic flux is excluded from its interior by the induction of surface currents[8].

not exceed the value of critical field H_c of the superconductor. As the resistance is zero the current will continue to flow with constant strength as long as the external field is kept constant and consequently the bulk of the superconductivity will stay field-free[1,8].

The exhibition of perfect diamagnetic property of superconductor can be shown as [2]:

$$B = \mu(H + M) \tag{2.3}$$

Where;M is magnetization, H is magnetic field and μ is permeability of free space from which the magnetic susceptibility χ can be found as:

$$\chi = \frac{M}{H} \tag{2.4}$$

By combining (2.3) and (2.4)

$$B = \mu H(1 + \chi) \tag{2.5}$$

If for a superconductor $B = 0$,it implies that $\chi = -1$. This realizes the superconductor is perfect diamagnetic[1-2].

2.3 Electron-Phonon Interaction

The usual treatment of ion movements in crystalline solids starts from the hypothesis that these movements are generally small-amplitude oscillations around the equilibrium positions that define the crystal structure[60]. This hypothesis is consistent with observed X-ray diffraction spectra consisting of very narrow lines[26]. These oscillations are commonly called lattice vibrations. Because interactions keep ions connected to one another, the vibrations are collective motions, and should be analyzed in the context of normal modes of the whole system[26-27]. The electron-phonon interaction causes superconductivity in many metals and influences the transport properties of every metal by describing coupled motions of electron and nuclei[26]. This model for the interaction explains classic physical phenomena, such as conventional superconductivity, and plays an important role in many active fields for instance, charge transport in molecular junctions[36]. The most natural environment in physics for implementing quantum gates is solid state systems where fermions (electrons) are subject of numerous interactions that concern and compromise quantum coherence. In particular, electron-electron and electron-phonon interactions are of central importance[27], because the attractive interaction between two electron is caused by the electron-phonon interaction supported by the discovery of isotopic effect on T_c showed that electron-phonon interaction plays an essential role in conventional superconductivity. The interaction between electrons and phonon by itself is strongly affected by the disorder of the electron system[28]. This is due to the attractive electron-electron interaction is mediated by phonon via the following mechanism[26,60]:

- An electron carries negative charge, and thus an electron will attract nearby nucleons. As a result, the spacing between the nucleons will be reduced around an electron (this is a lattice distortion). Because nucleons carrier of positive charge, smaller lattice spacing means that there is a higher positive charge density in this region near an electron.

- Electron mass is much smaller than nucleons, so electrons move much faster than nucleons. When electron flies away, the lattice distortion will not recover immediately (because nucleons move much slower). Locally, there is a higher density of positive charges here, which will attract other electrons.

- Combining the two facts mentioned above, we found that an electron will attract other electrons via lattice distortions. Because lattice distortions are described by phonon, this effect is known as phonon mediated attractions between two electrons.

2.4 The BCS theory of superconductivity

The basis of a quantum theory of superconductivity was laid by the classic 1957, papers of Bardeen, Cooper, and Schrieffer which is a BCS theory of superconductors for which they received the Nobel Prize in 1972[1]. According to the BCS theory, the interaction between electrons and phonon (the vibrational modes of the positive ions in the crystal lattice) causes a reduction in the Coulomb repulsion between electrons which is sufficient at low temperatures to provide a net long-range attraction[13]. This attraction causes the formation of bound pairs of remote electrons of opposite momentum and spin, the so-called Cooper pairs which is the central feature of the BCS theory[1,13]. A net attraction can be achieved if the electrons interact with each other via the motion of the crystal lattice as the lattice structure is momentarily deformed by a passing electron. The theory has been very successful in explaining the characteristic superconducting properties of zero resistance and flux expulsion[8]. Because one cannot reduce the momentum of a single cooper pair,without reducing the momenta of all other pairs by scattering[24]. The cooper pairs appear only at $T < T_c$ near the E_F [23]and the temperature dependent energy gap $\Delta(T)$ decreases momentarily with T from $\Delta(T = 0)$ to $\Delta(T = T_c) = 0$.

The BCS theory with wave theory along with a BCS wave function, which include[1,3]:

1. An attractive interaction between electrons can lead to a ground state separated from excited states by an energy gap (Δ), (The critical field, the thermal properties, and most of the electromagnetic properties are consequences of the energy gap).

2. The electron-lattice-electron interaction leads to an energy gap of the observed magnitude. The indirect interaction proceeds, when one electron interacts with the lattice and deforms it, a second electron sees the deformed lattice and adjusts itself to take advantage of the deformation to lower its energy. Thus the second electron interacts with the first electron via the lattice deformation.

3. The penetration depth and the coherence length emerge as natural consequences of the BCS theory. The London equation is obtained for magnetic fields that vary slowly in space. Thus the central phenomenon in superconductivity, the Meissner effect, is obtained in a natural way.

4. The criterion for the transition temperature of an element or alloy involves the electron density of orbitals$D(E_F)$ of one spin at the Fermi level and the electron-lattice interaction, U estimated from the electrical resistivity measure of electron phonon interaction in room temperature.

   For $D(E_F)U << 1$,The BCS theory predicts T_c as follow:

$$T_c = 1.14\Theta \exp(\frac{-1}{UD(E_F)}) \tag{2.6}$$

   Where; $\Theta = \sim\omega/K_B$ is the Debye temperature and $UD(E_F)$ is the coupling constant. In the same way the superconducting energy gap at $T = 0$ could be written as:

$$\Delta(0) = 2\sim\omega \exp(\frac{-1}{UD(E_F)}) \tag{2.7}$$

5. Magnetic flux through a superconducting ring is quantized and the effective unit of charge is 2e rather than e. The BCS ground state involves pairs of electrons; thus flux quantization in terms of the pair charge 2e is a consequence of the theory.

It is clear that T_c or the zero temperature variational parameter $\Delta(0)$ depends on material properties such as the phonon spectrum $\sim\omega$, the electronic structure $D(E_F)$ and the electron-ion coupling strength U[50]. Of various thermodynamic ratios it is possible to form $\frac{2\Delta(0)}{T^c} = 3.53$ for weak coupling which is the most relevant for conventional superconductors.
The temperature dependence of the gap $\Delta(T)$ near T_c can be computed numerically using the equation which is the universal function of T/T_c[3,41].

$$\frac{\Delta(T)}{\Delta(0)} \approx 1.74(1 - \frac{T}{T_c})^{\frac{1}{2}} \tag{2.8}$$

Where, $\Delta(0) = 1.76K_B T_c$,and $1 - \frac{T}{T_c} << 1$ in order to achieve this universal relation.

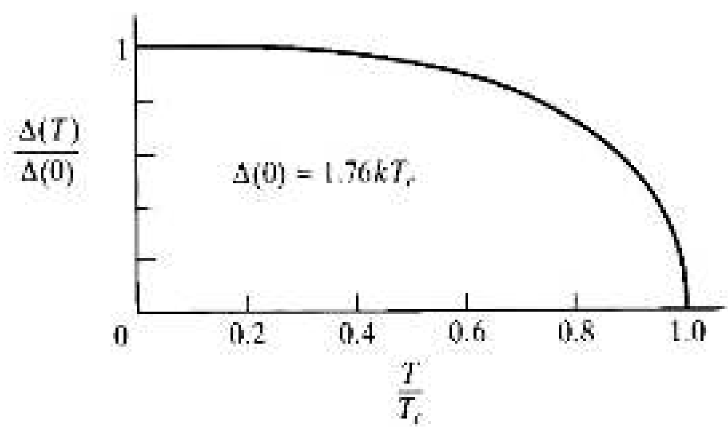

Figure 2.3: Behavior of the energy gap parameter $\Delta(T)$ for a superconductor in the BCS theory and weak coupling limit [3].

The energy gap decreases monotonically from its zero temperature value to zero at T_c as shown in Fig2.3. At very low temperatures Δ is nearly constant which can be physically interpreted as the fact that a significant number of quasi particles have to be excited before the energy gap value is effected by temperature variations.

2.5 London Equation

The electrodynamics equations of superconducting state were given by the two brothers H. London F. London in 1935 which was given the name London equations[1,3]. The current to the electromagnetic field around a superconductor can be related by the London equations[2-3]. The conventional electrodynamics equation applied to a perfect conductor leads to:

$$\frac{\partial B}{\partial t} = 0 \tag{2.9}$$

The discovery of Meissner effect realizes that superconductivity is a perfect diamagnetism ($B = 0$)[8,11]. In the superconducting state the current density (J_s) is directly proportional to the vector potential (A),where $B = \text{curl}A$[1]. From which the superconducting current density can be written as:

$$J_s = n_s q_s V_s \tag{2.10}$$

By taking the sum of the right hand side of equation(2.10) over charge carrier n_s we can write slightly the current density as:

$$J_s = \sum n_s q_s V_s \tag{2.11}$$

From Newton's law

$$\frac{mdV}{dt} = q_s E \tag{2.12}$$

Where; m=mass of super electron,V =velocity of charge carriers so that differentiating both sides of equation(2.11) and relating with equation(2.12) it yields:

$$\frac{dJ_s}{dt} = \underline{E} \sum \frac{n_s \; q_s}{m_s} \tag{2.13}$$

Due to Maxwell equation and taking the curl of both sides of (2.12):

$$\text{curl}J_s = -\frac{n_s \; q_s^2 B}{m_s} \tag{2.14}$$

This gives the value of J_s to be:

$$J_s = \frac{-n_s q_s A}{m_s} \tag{2.15}$$

Equation (2.15) is precisely London equation[1]. The London equation propose that the super current is proportional to the vector potential (curl$J_s = \mu_\circ J_s$), and taking curl on both sides we have;

$$\nabla^2 B = \frac{\mu_\circ n_s q_s^2 B}{m_s} \tag{2.16}$$

Equation (2.16) shows that B is not uniform inside the superconductor and the field gets exponentially damped as we go into the bulk material from the external surface[1-2]. If we define $\frac{\mu_\circ n_s q_s^2}{m_s} = \frac{1}{\lambda_L^2}$, the London penetration depth(λ_L) can be written as[1,4]:

$$\lambda_L = \left(\frac{m_s}{\mu_\circ n_s q_s^2}\right)^{\frac{1}{2}} \tag{2.17}$$

From Fig.2.4 it was observed that, when a superconductor is placed in a

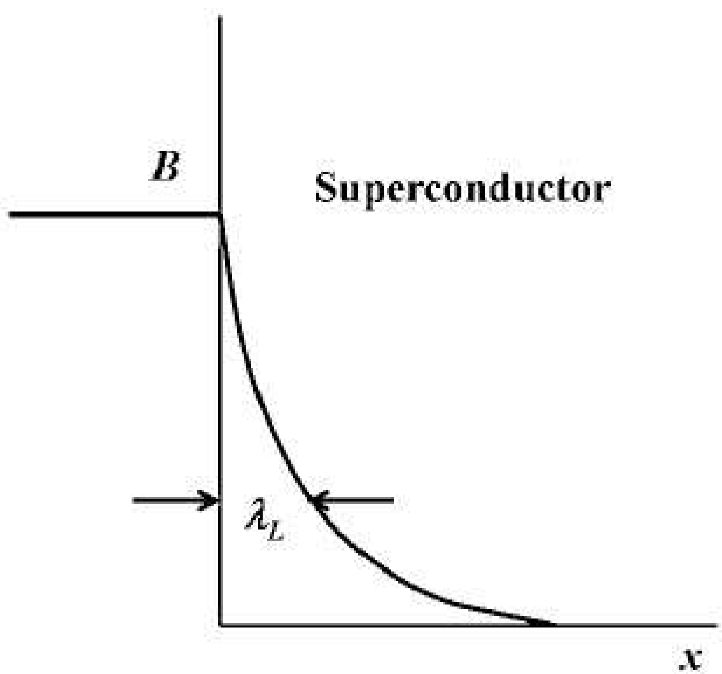

Figure 2.4: The magnetic field penetrates the superconductor within the range of λ_L as the Meissner effect is established in the superconductor which is thicker than λ_L [4]

weak external magnetic field, the field penetrates the superconductor only at a small distance of the London penetration depth λ_L, decaying exponentially to zero within the bulk of the material[1,3,4].

2.6 Ginzburg Landau Theory (GLT)

The GLT was proposed in 1950 which concentrates entirely on the superconducting electrons rather than an excitations[3,10]. Ginsburg and Landau were investigate the phenomenological theory of superconductor by using the order parameter $\psi(r)$ in order to introduce the concept of coherence length ξ [1,10,19]. The attraction of the GLT are the natural introduction of the coherence length ξ and the wave function used in the theory of the Josephson effect[1]. Through their theory, they introduce the constant ξ_{GL} known as Ginsburg Landau coherence length that is a measure of distance within which the superconducting electron concentration cannot change drastically in a spatially-varying magnetic field[1] which is given by:

$$\xi_{GL} = \left(\frac{\hbar^2}{2m|\alpha|}\right)^{\frac{1}{2}} \tag{2.18}$$

Ginsberg and Landau proposed that the ratio $\kappa = \frac{\lambda_L}{\xi_{GL}}$ is called Ginsberg-Landau parameter[4]. If there was a mixed states like $B_{c1} < B < B_{c2}$, based on the value of κ superconducting materials can be classified into type I and type II superconductors. Accordingly when;

1. $\kappa < \sqrt{\frac{1}{2}}$ the material is type I superconductor.
2. $\kappa > \sqrt{\frac{1}{2}}$ the material is type II superconductor.

2.7 Magnetic Properties of Type I and Type II Superconductors

In section 2.6 we explained the type I and type II superconductors based on the value of κ. We can also distinguish superconductors into type I type II on the basis of their magnetic properties. Type I superconductors(pure superconductors) excludes a magnetic field until superconductivity is destroyed suddenly and field penetrates completely [1,3,11]. The elements aluminum, mercury, lead, tin and indium are some examples of type I superconductors [1,11,12]. Type II superconductors(superconducting alloys) are characterized by two critical fields H_{c1} and H_{c2}[1,3,11]. Below H_{c1} these substances are in the Meissner phase with complete field expulsion while in the range, $H_{c1} < H < H_{c2}$ a type II superconductor enters the mixed phase in which the magnetic field can penetrate the bulk material in the form of flux tubes[11].Above H_{c2}, the material becomes normal state. Nb_3Sn, $YBa_2Cu_30_6$, $Tl_2Sr_2Ca_3CuO_{10}$ and MgB_2 are some instances of type II superconductors [12].

In fig.2.5, when type I superconductor is placed in the magnetic field it sud-

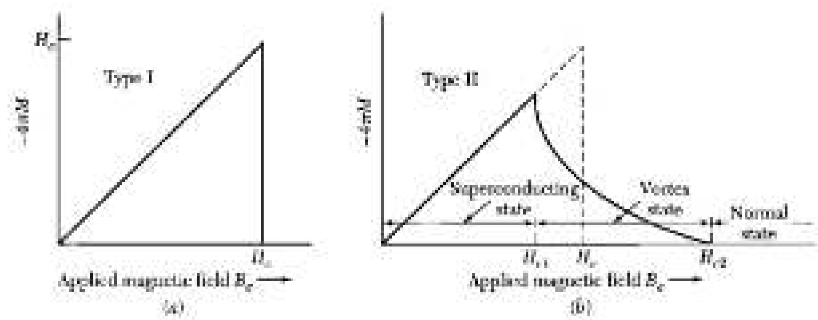

Figure 2.5: (a) Magnetization versus applied magnetic field for a bulk snpercooductor exhibiting a complete Meissner effect (perfect diamagnetism). (b) Superconducting magnetization curve of a type I1 superconductor. The flux starts to penetrate the specimen at a field H_{c1}, lower than the thermodynamic critical field H_c[1].

denly looses it's superconductivity at critical magnetic field H_c. After H_c type I superconductor will become conductor[29]. But ,when type II superconductor is placed in the magnetic field unlike type I it gradually looses it's superconductivity. Type II superconductors start to loose their superconductivity at lower critical magnetic field H_{c1} and completely loose their superconductivity at upper critical magnetic field H_{c2}. The vortex state (intermediate state)is found between H_{c1} and H_{c2} for type II superconductors and after H_{c2} the material becomes the normal state.

2.8 Overview of Fe-based superconductors

The superconducting phenomenon is known to occur in about two thousand kinds of materials, including elements, alloys, various metallic compounds, and organic materials [4]. Of various metallic compounds, Fe-based compounds are available at higher T_c as superconducting materials. After the investigation of $La-O-Fe-P$ superconductors, the ongoing search for new superconductors has yielded as a family of $LaO_{1-x}F_xFeAs$ oxypnictides composed of altering $LaO_{1-x}F_x$ and $FeAs$ layers with T_c of 26K in 2008 ,and this T_c value raised to 56K by replacing La with Sr and Sm[4]. This rapid sequence of discoveries captured the attention of the high-temperature superconductivity community[37]. A large variety of other iron pnictides and chalcogenides have been shown to be superconductors with some reports of T_c as high as 100K[20]. The symmetry and the structure of the superconducting gap in FeSCs, their evolution and possible change with doping are currently subjects of intensive debates in the condensed matter community[6,7,9]. The basic crystallographic elements of the FeSC is the $FeAs$ (where instead of As one can also have P, Se or Te)[37]. Most of the researchers believe that the superconductivity in FeSC is of electron origin and results from the screened coulomb interaction enhanced at particular momenta due to strong magnetic fluctuations or orbitals fluctuation[6-7]. It is generally agreed that magnetism plays an important role in superconductivity of FeSC[20].

There are a large number of Fe-based compounds which may broadly be classified into two categories Fe-pnictides $FePn$ and Fe-chalcogenides $FeCh$ [61]. The former can further be classified into four categories whereas the later into two, giving rise to a total of six categories of Fe-based materials based on their chemical composition and crystal symmetry which are presented as follow[44,61].

Families	Formula	Appropriate elements for combination
1111	**R**FeAsO	La, Ce, Sm, Nd
122	**A**Fe_2As_2	Ba, Ca, Sr
111	**A**FeAs	Na, Li
21311(or 42622)	$Sr_2\mathbf{M}O_3Fe\mathbf{Pn}$	**M** = Sc, V, Cr and **Pn** = P, As
11	Fe**M**	Se, Te
122*	$\mathbf{A}_{0.8}Fe_{1.6}Se_2$	K, Rb, Cs, Tl

2.9 Antiferromagnetic Order

The discovery of a number of different high-T_c superconducting materials include hole-doped $La_{2-x}Sr_xCuO_{4+\delta}$ (LSCO), $YBa_2Cu_3O_{6+\delta}$ (YBCO), $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO), and $Tl_2Ba_2CuO_{6+\delta}$(TBCO) materials, and electron-doped $Nd_{2-x}Ce_xCuO_4$ (NCCO)[30]. All these materials have two-dimensional CuO_2 planes and display an AF insulating phase at half filling. The magnetic properties of this insulating phase are well approximated by Heisenberg model with spin $S = 1/2$ and an AF exchange constant $J \sim 100meV$ [31]. On the other hand, the recent discovery of a new Fe-based superconducting system $A_xFe_{2-y}Se_2$ (A, alkaline metals or Tl, $x \leq 1$) with T_c over 30 K has attracted considerable attention[32]. This would happen until the two electronic phases were believed to play a vital role in iron-based superconductivity where,the electronic phases are stripe or double-stripe-type AF ordering at a non doped $Fe-3d$ state and a mott insulator at a hole-doped $Fe-3d$ state[33]. In this case a non doped $Fe-3d$ observed at ambient pressure for the arsenides and telluride, while under high pressures for the selenides, and the AF fluctuations are a promising candidate for the pairing glue leading to superconductivity[32]. But, a hole-doped $Fe-3d$ confirmed recently in effectively hole-doped $Na(Fe^{3+}_{0.5}Cu^{+}_{0.5})As$ explains the asymmetric response of the T_c and electron correlation to hole and electron doping, where the hole doping (electron doping) into the $Fe-3d$ state tends to enhance (reduce) the T_c and the degree of electron correlation, because the system approaches (goes away from) the half-filled $Fe-3d$ state [32-33].

In general, the superconductivity has been suggested to arise from a magnetic coupling between electron and hole pockets at the FS [34]. Such a pairing

interaction mediated by magnetic excitations (spin waves) can lead to a multi-band superconductivity with a sign reversal between the electron pocket and the hole pocket, represented by the s wave symmetry.
The theoretical calculation for parent LiF eAs shows that the FS of parent LiF eAs is composed of two hole cylinders at the zone center and two electron cylinders at the zone corner[35]. The hole and electron Fermi surfaces are also nearly nested that leads to the formation of long range magnetic order that results the wave symmetry type anti ferromagnetic fluctuation state is the favorable state for LiFeAs in terms of energy[20,33,35].

2.10 Application of Superconductivity

It was believed on theoretical grounds that there would be no superconductors above 30K[21]. But after the discovery of high temperature superconductivity by Bednorz and Müller in 1986, it was reported that the superconductivity of $(LaA)_2CuO_4$ in doped lanthanum copper oxides occurred at temperatures up to 38K[4]. Where, A is Ba or Sr. This is a tremendous excitement, since 38K was above the ceiling of 30K for superconductivity. The investigation of HTSC was not the end, the compound yttrium barium copper oxide $YBa_2Cu_3O_7$ has been found to be superconductor up to 92K[24].Immediately bismuth strontium calcium copper oxide $Bi_2Sr_2Ca_2Cu_3O_{10}$ at T_c of 110K and thallium barium calcium copper oxide $Tl_2Ba_2Ca_2Cu_3O_{10}$ at T_c of 125K exhibit superconductivity turn by turn[4,24].

Two decades after the discovery of HTSCs, practical superconducting wires made of these materials are now being manufactured, and trials of electrical and industrial applications including a train supported by magnetic levitation, a transmission line, a ship's engine, radiation-free magnetic resonance imaging in medical diagnosis and many others are being implemented[21,24].
For instance, in case of transportation, maglev trains have attained top speeds in excess of 500kmph. Some transportation experts believe that maglev trains could modernize transportation in the 21st century in much the same way that airplanes modernized the 20th century transportation system[24,25]. At

present, maglev train lines operating in Japan, Germany, and China make use of low temperature superconductor technology[21,24]. Of course the application of HTSCs to maglev trains are under research which will expected in lower costs and stability[21]. In general superconductivity has played a key role throughout the past century in expanding the frontiers of human knowledge, and today these materials continue to offer important new tools to expand our understanding of the natural world and potentially foster new energy technologies[25].

2.11 Behaviors of LiFeAs

2.11.1 LiFeAs as Iron Based Superconductor

After the original discovery of superconductivity in $LaOFeAs$[48] with a superconducting transition temperature $T_c = 26K$, the investigation of FeSCs has lead to the discovery of several classes of compounds that all display a high-temperature superconductivity[48]. Despite the fact that the different lattice structures can lead to significant differences in the electronic structure[47,49]. A large number of quaternary iron-oxypnictides $RFeAsO (R = Ce, Pr, Nd, and Sm)$, often called '1111' systems, were found to be superconducting with T_c up to 55K for $SmFeAs(O, F)$ series[48]. In a search for the mechanism of superconducting pairing in FeSC, $LiFeAs$ is, apparently a key compound[47]. This FeSC has attracted recently much attention due to its unusual properties compared to other superconducting iron pnictides. Since it reveals the classical isotropic superconducting gap[44], it is expected that the pairing glue is provided by phonon[45]. $LiFeAs$ is a very remarkable member in the family of FeSC (mainly 111 family) containing $FeAs$ layer with an average iron valence Fe^{2+}[2,18,19] and it is metallic superconductor with itinerant electrons. The magnetic exchange interactions in this compound is AF fluctuation[5,12,20]. Because of the spin-density wave ordering and the structural transition seen in the parent compounds of the "1111" and the "122" systems are not present in LiFeAs, that is why unlike other stoichiometric iron-arsenide compounds LiFeAs is an intrinsic superconductor[19,22]. This compound has relatively high transition temperature of 18K without the need for carrier doping or applications of pressure to induce superconductivity. Moreover its electronic structure is quasi-two dimensional (2D) [37] and supports superconductivity in the absence of any notable FS nesting or static magnetism. Figure 2.6 shows a typical temperature dependence of the resistivity of LiF eAs as it's transition occurs at 18K.

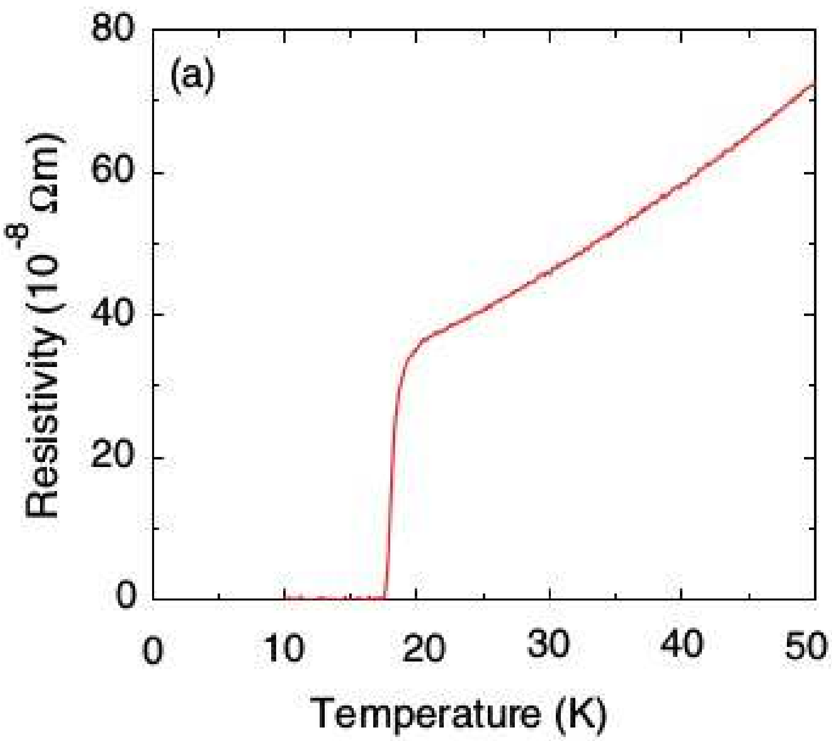

Figure 2.6: (Color online) Temperature dependence of the resistivity of a single crystal of LiF eAs whose transition temperature T_c is 18K [46].

In addition; it reveals a perfectly two-dimensional $Fe - 3d_{xy}$ electronic band which was well separated in momentum space from other bands[42-43]. The band structure calculation shows that the FS of LiF eAs consists of three hole-like FSs around the Γ-point, and two electron-like ones at the corner of the Brillouin zone[45].

2.11.2 Crystal Structure of LiFeAs

A crystal is formed by adding atoms in a constant environment[1]. Crystal structure is also a structure consists of identical copies of the same physical unit cell called the basis; located at all the points of a Bravais lattice[10]. The superconducting iron arsenide system LiFeAs (termed"111") crystallizes into a Cu_2Sb type tetragonal structure[49] containing FeAs layer with an average iron valence Fe^{+2} like those for "1111" or "122" parent compounds.

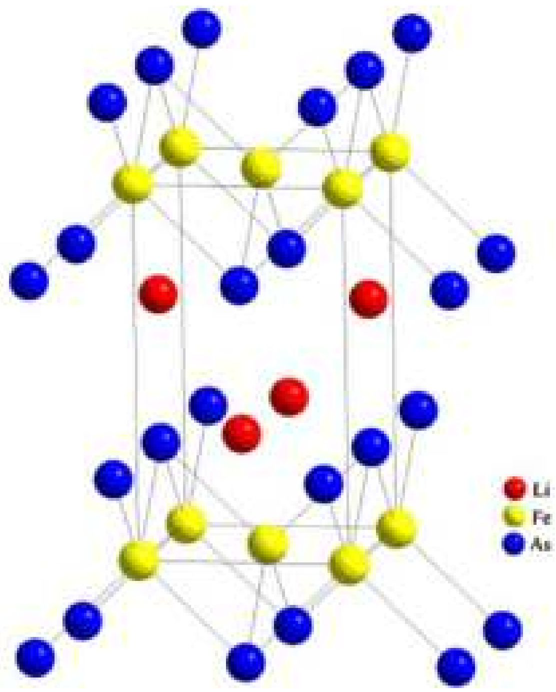

Figure 2.7: Crystal structure of LiFeAs characterized by tetragonal layer. The atomic lattice parameters are for Li, As : a = 3.8 and for Fe : a = 2.7. In this figure, the red (gray) spheres are Li atoms, the blue (dark gray) spheres are As atoms, and the yellow (light gray) spheres are Fe atoms[17].

From Fig.2.7 an edge-sharing $FeAs_4$ tetragonal layer in LiFeAs consists of one layer of Fe sandwiched between two layers of As[17]. Two layers of Li atoms are interlaced between FeAs and form the neutral cleaving plane without surface reconstruction. This helps to apply scanning tunneling microscope (STM) and angle resolved photoelectric spectroscopy (ARPES) in order to capture the intrinsic properties of LiFeAs[46].

2.11.3 Band Structure of LiF eAs

The LiF eAs phase belongs to a wide family of compounds with the tetragonal structure and can be considered as the "first representative of the third group (type 111)" of the new FeAs superconductors[56]. Unlike other pnictides, such as BaF e_2As_2 and N aF eAs, LiF eAs is a superconductor in its stoichiometric form and any chemical substitution on the Fe site (with Co or Ni, for instance) causes a reduction in the transition temperature T_c[57]. In contrast with other systems, no ordered magnetic phase or structural transition has yet been observed in LiF eAs[56-57]. The electron nature of the carriers and superconductivity in undoped LiF eAs allowed researchers to thought the detailed band-structure calculations and further experiments[58]. Thus; the detail of band-structure calculations of this compound resolved by density functional theory would be discussed as follow:

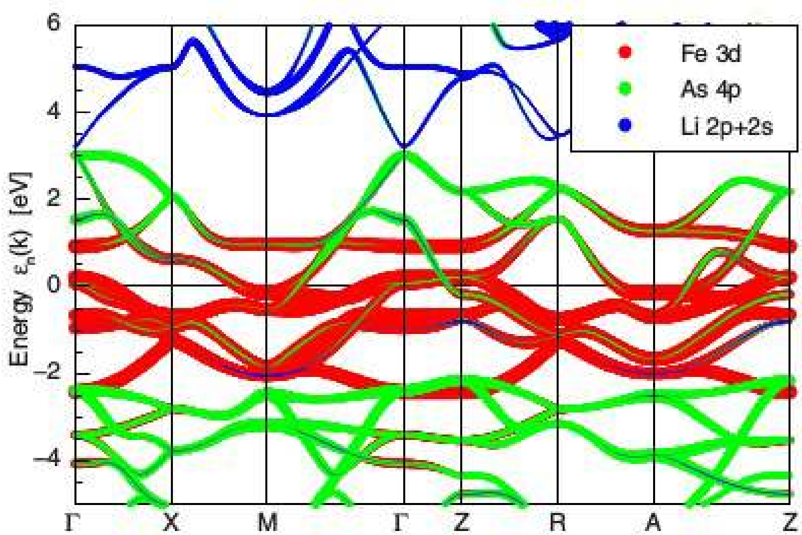

Figure 2.8: Band structure of bulk LiFeAs. The F e 3d bands (red color) together with some hybridization of the As 4p states(green color)dominate the entire low-energy spectrum and the strong Z dispersion of Li bands(blue color) couples to As at higher energies and to F e at lower-energies[59].

From band structure of LiF eAs one can summarizes that[56]:

- The valence band for this compound is comprised primarily of the 3d states of F e and 4p states of As.
- It's lower edge includes the overlapping (hybrid) 3d states of F e and 4p states of As forming the covalent bond F e − As bonds in the F eAs_4.

- The near-Fermi region consists primarily of the 3d states of F e, that make the main contribution to the total density of states at the FL, which are responsible for the conducting properties of the system.

As the superconductor LiF eAs behaves non-stable magnetic property, the pairing mechanism is not only electron-phonon interaction, but also the interaction between the electron band and incipient band can be thought of as being spin fluctuation[14].

2.12 Electron pairing in the presence incipient band

The standard paradigm for $s_{\pm}$ pairing in FeSC relies on the existence of a hole-like FS near $K = 0$ [14-15], and electron-like FS near $K = (\pi, 0)$ in the first Brillouin zone, and symmetry related points. Usual arguments leading to $s_{\pm}$ pairing by repulsive interactions acting between hole and electron pockets must break down[16]. Beginning in 2010 with the discovery of superconducting in the alkali-intercalated FeSe materials[14] the paradigm was challenged by the subsequent remarkable discover that all hole bands in the materials with optimal T_c greater than 40K below the Fermi level. Several group pointed out that the hybridization forced by 122 crystal structure can lead to the possibility of a nova ”bonding-anti bonding” state with opposite signs on the two M-centered hybridized electron pocket in the second Brillouin zone[14-15]. The repulsive interactions at the Fermi level remained among the electron FS pockets, and could lead to $d-$wave pairing with critical significant temperatures[14].

Since the pairing in an $s_{\pm}$channel with sign changing gap was quite competitive[17] and the hole band was 90mev below the FL and this shows, there was an indication of the existence of spin fluctuations which results incipient $s_{\pm}$ wave consideration along with two d-wave state[14]. As a result a more subtle s- wave state that changed sign between two hybridized electron pockets in the 2-Fe zone as a possible candidate for pairing in this materials, it did not receive a great deal of attention. This is probably because of the general feeling in the community that incipient bands (incipient means bands away from the FL but within a 'pairing' cutoff energy) do not play an important role in superconductivity,and contrary to that in the presence of well-stabilized superconducting, an incipient band can significantly enhance T_c as well as the induced superconducting gap on the incipient band can be large[14]. This includes typical bulk FeSCs like LiF eAs where a significant gap on an incipient band has been seen experimentally.

2.13 Green's Functions Method in Superconductivity

The Green's function is a mathematical tool used as a shortcut through problems on differential equations[38]. It is a method which is widely used in physics in general and specifically in condensed matter physics for the theoretical investigation of many-body systems. However, this classical way of solving the problems is hardly needed when looking into the superconductor problem[26]. The Green functions are defined by a particle's initial and final space-time r^0t^0 and rt, as well as its initial and final spin σ^0 and σ[39]. They give the probability for a particle to propagate from r^0t^0 to rt.

There are six types of Green functions among these, the double-time thermodynamic retarded and advanced Green's functions introduced by Bogoliubov and Tyablikov[40] were found to be an efficient tool in investigation of quasi particle spectra in the theory of many-body systems and in the superconductivity theory, in particular. We introduce these two Greens functions from which many important physical quantities are more easily extracted[63]. For times $t > t^0$ and $t < t^0$ the retarded and advanced Greens functions are respectively defined for fermions as follow[39,62]:

$$G^R(t, t^0) = -i\theta(t - t^0) << [A(t), B(t^0)] >> \tag{2.19}$$

$$G^A(t, t^0) = +i\theta(t^0 - t) << [A(t), B(t^0)] >> \tag{2.20}$$

In these definitions of Green's functions; $A(t)$ and $B(t')$ are time-dependent Heisenberg operators, $[A, B] = AB + BA$ is the anti commutator which is appropriate for fermions, and $<< \ldots >>$ denotes averaging over equilibrium state. The step function is also given by:

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

The commutation and anti-commutation relations of operators involved in Green's function should be well treated in order to handle the problem .This is possible by using the Leibniz rules for commutators and anti-commutators in case of multiple fermionic modes which are listed below[64-65]:

$$\begin{aligned} [A, BC] &= [A, B]C + B[A, C] = \{A, B\}C - B\{A, C\}, \\ [AB, C] &= A[B, C] + [A, C]B = A\{B, C\} - \{A, C\}B, \\ \{A, BC\} &= [A, B]C + B\{A, C\} = \{A, B\}C - B[A, C], \\ \{AB, C\} &= A[B, C] + \{A, C\}B = A\{B, C\} - [A, C]B \end{aligned} \tag{2.21}$$

Chapter 3

Methodology

3.1 Mathematical Formulation

To study the superconductivity of LiFeAs due to incipient band, the superconducting parameters; the superconducting energy gap at zero temperature ($\Delta(0)$) and transition temperature (T_c) has been calculated and approximated. In order to do so we applied Green's Function. We try to calculate these superconducting parameters using the suitable Hamiltonian and compare those calculated value with experimental values for the LiF eAs superconductor. The model Hamiltonian representing superconductivity of LiF eAs due to incipient band is arising from the direct and indirect electron interaction which are reduced to the BCS model.

$$H = H_{\circ} + H^{0} \tag{3.1}$$

$$H_{\circ} = \sum_{k\sigma} {}_{k} a^{\dagger}_{k\sigma} a_{k\sigma} + \sum_{m\sigma} {}_{m} c^{\dagger}_{m\sigma} c_{m\sigma} \tag{3.2}$$

Where H^{0} have the form:

$$H^{0} = H^{0}_{1} + H^{0}_{2} \tag{3.3}$$

$$H^{0}_{1} = \sum_{kk^{0}} V_{kk^{0}} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{-k^{0}\downarrow} a_{k^{0}\uparrow} \tag{3.4}$$

$$H^{0}_{2} = \sum_{km} \alpha_{km} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} c_{-m^{0}\downarrow} c_{m^{0}\uparrow} + \sum_{km} \alpha^{*}_{km} a_{-k^{0}\downarrow} a_{k^{0}\uparrow} c^{\dagger}_{m\,\shortmid} c^{\dagger}_{-m\downarrow} \tag{3.5}$$

Where, $H_{\circ}$ is the Hamiltonian of free electron and localized electron, H^{0}_{1} is the Hamiltonian of electron-electron interaction through fermion exchange, and H^{0}_{2} is the interaction term between conduction electron and localized electron due to incipient band with some coupling constant α. ϵ_k and ϵ_m are the band energies (excitation energies) of conduction electron and localized electro respectively measured from Fermi energy. $a^{\dagger}_{k\sigma}(a_{k\sigma})$ and $c^{\dagger}_{m\sigma}(c_{m\sigma})$ are creation and annihilation operators of conduction electron and localized electron respectively.

Thus; the overall model Hamiltonian representing our work is the sum of the Hamiltonians that looks like :

$$H = \sum_{k\sigma} \epsilon_k a^{\dagger}_{k\sigma} a_{k\sigma} + \sum_{m\sigma} \epsilon_m c^{\dagger}_{m\sigma} c_{m\sigma} + \sum_{kk'} V_{kk'} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{-k'\downarrow} a_{k'\uparrow} + \sum_{km} \alpha_{km} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} c_{-m'\downarrow} c_{m'\uparrow} + \sum_{km} \alpha^{*}_{km} a_{-k'\downarrow} a_{k'\uparrow} c^{\dagger}_{m\uparrow} c^{\dagger}_{-m\downarrow} \quad (3.6)$$

Applying the retarded green's function G^R, we can formulate the EOM by using $a^{\dagger}$ and a as follow:

$$\omega \ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg = \langle [a_{k\uparrow}, a^{\dagger}_{k\uparrow}] \rangle + \ll [a_{k\uparrow}, H]; a^{\dagger}_{k\uparrow} \gg \quad (3.7)$$

The commutation relation would likely applied to the second term of the right hand side of equation (3.7) based on the hamiltonian given in equation (3.6).

$$[a_{k\uparrow}, H] = [a_{k\uparrow}, H_\circ + H'_1 + H'_2] \quad (3.8)$$

$$= [a_{k\uparrow}, H_\circ] + [a_{k\uparrow}, H'_1] + [a_{k\uparrow}, H'_2] \quad (3.9)$$

We can plausibly found the values of commutation relation of fermions using Leibniz rule for commutators and anti commutators of the first term of the right hand side of equation (3.7) and equation (3.9) as follow as long as the anti commutation relation of fermion is defined first.

$$\begin{aligned} [a_{k\uparrow}, a^{\dagger}_{k\uparrow}] &= \delta_{k\uparrow} = 1 \\ [a_{k\uparrow}, a_{k\uparrow}] &= 0 \\ [a^{\dagger}_{k\uparrow}, a^{\dagger}_{k\uparrow}] &= 0 \end{aligned} \quad (3.10)$$

$$[a_{k\uparrow}, H_{\circ}] = [a_{k\uparrow}, \sum {}_k a^{\dagger}_{k\sigma} a_{k\sigma} + \sum {}_m c^{\dagger}_{m\sigma} c_{m\sigma}] \quad (3.11)$$

$$= {}_k a_{k\uparrow} \quad (3.12)$$

$$[a_{k\uparrow}, H^{0}_{1}] = [a_{k\uparrow}, \sum_{kk^{0}} V_{kk^{0}} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{-k^{0}\downarrow} a_{k^{0}\uparrow}] \quad (3.13)$$

$$= \sum_{k} V [a_{k\uparrow}, a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{-k^{0}\downarrow} a_{k^{0}\uparrow}] \quad (3.14)$$

$$= \sum_{k} V a^{\dagger}_{-k\downarrow} a_{-k^{0}\downarrow} a_{k^{0}\uparrow} \quad (3.15)$$

$$[a_{k\uparrow}, H^{0}_{2}] = [a_{k\uparrow}, \sum_{km} \alpha_{km} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} c_{m^{0}\uparrow} c_{-m^{0}\downarrow}$$
$$+ \sum_{km} \alpha^{*}_{km} a_{-k^{0}\downarrow} a_{k^{0}\uparrow} c^{\dagger}_{m\uparrow} c^{\dagger}_{-m\downarrow}] \quad (3.16)$$

$$= \sum_{km} \alpha_{km} a^{\dagger}_{-k\downarrow} c_{m^{0}\uparrow} c_{-m^{0}\downarrow} \quad (3.17)$$

Inserting equations (3.10),(3.12),(3.15), and (3.17) into equation (3.7) it yields that:

$$\omega << a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> = 1 + << {}_k a_{k\uparrow} + \sum V a^{\dagger}_{-k\downarrow} a_{-k^{0}\downarrow} a_{k^{0}\uparrow}$$
$$+ \sum_{km} \alpha_{km} a^{\dagger}_{-k\downarrow} c_{m^{0}\uparrow} c_{-m^{0}\downarrow}; a^{\dagger}_{k\uparrow} >> \quad (3.18)$$

$$= 1 + {}_k << a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> + << \sum V a^{\dagger}_{-k\downarrow} a_{-k^{0}\downarrow} a_{k^{0}\uparrow}, a^{\dagger}_{k\uparrow}$$
$$+ << \sum_{km} \alpha_{km} a^{\dagger}_{-k\downarrow} c_{m^{0}\uparrow} c_{-m^{0}\downarrow}, a^{\dagger}_{k\uparrow} >> \quad (3.19)$$

We can write the higher order Green's Function into lower Green's Function using decoupling mechanism.

$$<< \sum V a^{\dagger}_{-k\downarrow} a_{-k^{0}\downarrow} a_{k^{0}\uparrow}, a\dagger_{k^{0}\uparrow} >> = \sum V < a_{-k^{0}\downarrow} a_{k^{0}\uparrow} >< < a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> \quad (3.20)$$

$$= \Delta << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> \quad (3.21)$$

Where, Δ is the superconducting order parameter and using the same procedure we have:

$$<< \sum_{km} \alpha_{km} a^{\dagger}_{-k\downarrow} c_{m'\uparrow} c_{-m'\downarrow}, a^{\dagger}_{k\uparrow} >> \; = \; \sum \alpha < c_{m'\uparrow} c_{-m'\downarrow} >< < a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> \tag{3.22}$$

$$= \vartheta << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> \tag{3.23}$$

Here ϑ stands for magnetic order parameter. Through substituting equation (3.21) and equation (3.23) into equation (3.19) it would resulted that:

$$\omega << a_{k\uparrow}, a^{\dagger}_{k\uparrow} >>= 1 + {}_{k} << a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> + \Delta << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> + \vartheta << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> \tag{3.24}$$

By rearranging equation (3.24), the EOM reads:

$$(\omega - {}_{k}) << a_{k\uparrow}, a^{\dagger}_{k\uparrow} >>= 1 + (\Delta + \vartheta) << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> \tag{3.25}$$

Following the same procedure as we have did above, we ca also determine EOM by using the higher order Green's Function $<< a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >>$.

$$\omega << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> \; = \; < [a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow}] > + << [a^{\dagger}_{-k\downarrow}, H]; a^{\dagger}_{k\uparrow} >> \tag{3.26}$$

$$= << [a^{\dagger}_{-k\downarrow}, H_{\circ} + H'_{1} + H'_{2}]; a^{\dagger}_{k\uparrow} >> \tag{3.27}$$

Each values of the commutation for fermions of equation (3.27) should be simplified as follow:

$$[a^{\dagger}_{-k\downarrow}, H_{\circ}] \; = \; [a^{\dagger}_{-k\downarrow}, \sum_{k\sigma} {}_{k} a^{\dagger}_{k\sigma} a_{k\sigma} + \sum_{m\sigma} {}_{m} c^{\dagger}_{m\sigma} c_{m\sigma}] \tag{3.28}$$

$$= - {}_{k} a^{\dagger}_{-k\downarrow} \tag{3.29}$$

$$[a^{\dagger}_{-k\downarrow}, H^{0}_{1}] = [a^{\dagger}_{-k\downarrow}, \sum_{k} V_k a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{-k^{0}\downarrow} a_{k^{0}\uparrow}] \tag{3.30}$$

$$= \sum_{k} V\, a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{k\uparrow} \tag{3.31}$$

$$[a^{\dagger}_{-k\downarrow}, H^{0}_{2}] = [a^{\dagger}_{-k\downarrow}, \sum_{km} \alpha_{km} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} c_{-m^{0}\downarrow} c_{m^{0}\uparrow} + \sum_{km} \alpha^{*}_{km}\, a_{-k^{0}\downarrow} a_{k^{0}\uparrow} c^{\dagger}_{m\uparrow} c^{\dagger}_{-m\downarrow}] \tag{3.32}$$

$$= \sum_{km} \alpha^{*}\, a_{k\uparrow} c^{\dagger}_{m\uparrow} c^{\dagger}_{-m\downarrow} \tag{3.33}$$

Inserting equations (3.29), (3.31), and (3.33) into equation (3.27) it yields:

$$\omega << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> = -\,{}_{k} << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> + << \sum_{k} V\, a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> + << \sum_{km} \alpha^{*}\, a_{k\uparrow} c^{\dagger}_{m\uparrow} c^{\dagger}_{-m\downarrow}, a^{\dagger}_{k\uparrow} >> \tag{3.34}$$

By applying decoupling mechanism, we can write equation (3.34) as a simplified form of EOM.

$$<< \sum_{k} V\, a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> = \sum_{k} V < a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} >< < a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> \tag{3.35}$$

$$= \Delta << a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> \tag{3.36}$$

$$<< \sum_{km} \alpha^{*}\, c^{\dagger}_{m\uparrow} c^{\dagger}_{-m\downarrow} a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> = \sum_{km} \alpha^{*} < c^{\dagger}_{m\uparrow} c^{\dagger}_{-m\downarrow} >< < a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> \tag{3.37}$$

$$= \vartheta << a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> \tag{3.38}$$

$$(\omega + {}_{k}) << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >>= (\Delta + \vartheta) << a_{k\uparrow}, a^{\dagger}_{k\uparrow} >> \tag{3.39}$$

We wish to combine equations (3.25) and (3.39) in order to write the overall EOM, which is the basis for calculating superconducting parameters. From equation(3.25) we have, $<< a_{k\uparrow}, a^{\dagger}_{k\uparrow} >>= \frac{1}{\omega - {}_{k}} + \frac{\Delta+\vartheta}{\omega - {}_{k}} << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >>$, and inserting this into equation (3.39) and rearranging gives the EOM for the system which looks like the following.

$$<< a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >>= \frac{\Delta + \vartheta}{\omega^2 - {}^{2}_{k} - (\Delta + \vartheta)^2} \tag{3.40}$$

3.1.1 The Superconducting Energy Gap

The superconducting energy gap (Δ) is the energy difference between the ground state of superconductors and the energy of lowest quasi-particle excitation. Or it is the energy gap corresponds to the energy difference between the electrons in the superconducting and normal states. To calculate the superconducting energy gap at a temperature of 0K, let's express Δ in terms of EOM.

$$\Delta = -\frac{V}{\beta} \sum_{kn} << a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} >> \tag{3.41}$$

V is negative because according to BCS theory the basis for superconductivity is that electrons form pairs, called Cooper pairs, due to an effective, attractive interaction between them which means that V is a pairing potential arising from electron-phonon interaction[3,26]. β is the quasi-particle operator corresponds to excitation to BCS ground state or it is the inverse of temperature.
If the attractive interaction is effective (or finite) for the region $-\tilde{\omega} < 0 < \tilde{\omega}$ and assuming that the density of states $N(o)$ is constant at the Fermi level; over this range Δ becomes:

$$\Delta = -\frac{2V}{\beta} N(o) \sum_{n} \int_{0}^{\tilde{\omega}} \left(\frac{\Delta + \vartheta}{\omega^2 - {}^{2}_{k} - (\Delta + \vartheta)^2}\right) d \tag{3.42}$$

Where, $\tilde{\omega}$ is Debye energy and changing $\omega \longrightarrow i\omega_n$ and use the Matsubara frequency for fermion (ω_n) given by, $\omega_n = \frac{(2n+1)\pi}{\beta}$ from which ω_n^2 could be expressible as:

$$\omega_n^2 = -\frac{(2n+1)^2\pi^2}{\beta^2} \tag{3.43}$$

Putting equation (3.43) into equation (3.42), we can write the value of Δ.

$$\Delta = -\frac{2V}{\beta} N(o) \sum_n \int_0^{\hbar\omega} \frac{\Delta + \vartheta}{-((2n+1)^2\pi^2 + ({}_k^2 + (\Delta+\vartheta)^2)\beta^2)} d \tag{3.44}$$

$$= 2N(o)V\beta \sum_n \int_0^{\hbar\omega} \frac{\Delta + \vartheta}{(2n+1)^2\pi^2 + E^2\beta^2} d \tag{3.45}$$

Where $E^2 = {}_k^2 + (\Delta+\vartheta)^2$, and using the fact that

$$\frac{1}{2x}\tanh\frac{x}{2} = \sum_n \frac{}{(2n+1)^2\pi^2 + x^2}$$

We can write equation (3.45) as follow.

$$\Delta = 2N(o)V\beta \int_0^{\hbar\omega} (\frac{\Delta+\vartheta}{2E}\tanh\frac{\beta E}{2}) d \tag{3.46}$$

Let, $\lambda = N(o)V$ that represents the coupling constant between conduction electron and localized electron so that equation (3.46) can be written as:

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega} d \frac{\Delta+\vartheta}{\sqrt{{}_k^2 + (\Delta+\vartheta)^2}} \tanh\frac{\beta\sqrt{{}_k^2 + (\Delta+\vartheta)^2}}{2} \tag{3.47}$$

From equation (3.47), it is possible to calculate the superconducting energy gap at 0K. This time as $T \longrightarrow 0K$, $\beta \longrightarrow \infty$, which helps us to approximate $\tanh\frac{\beta\sqrt{{}_k^2+(\Delta+\vartheta)^2}}{2} \longrightarrow 1$, and to reduce the equation.

$$\frac{\Delta}{\lambda(\Delta+\vartheta)} = \int_0^{\hbar\omega} \frac{1}{\sqrt{{}_k^2 + (\Delta+\vartheta)^2}} d \tag{3.48}$$

From the integral pattern of $\int \frac{1}{\sqrt{x^2+a^2}}dx = \ln|x + \sqrt{x^2+a^2}|$, an integral of equation (3.48) simplified and gives:

$$\frac{1}{\lambda(1+\frac{\vartheta}{\Delta})} = \ln|\hbar\omega + \sqrt{(\hbar\omega)^2 + (\Delta+\vartheta)^2}| - \ln(\Delta+\vartheta) \tag{3.49}$$

$$= \ln\frac{(\hbar\omega + \sqrt{(\hbar\omega)^2 + (\Delta+\vartheta)^2})}{\Delta+\vartheta} \tag{3.50}$$

After rearranging the value of $\Delta + \vartheta$ reads as follow.

$$\Delta + \vartheta = 2\hbar\omega \exp\left(-\frac{1}{\lambda(1 + \frac{\vartheta}{\Delta})}\right) \tag{3.51}$$

The value of Δ is the same with the BCS model with additional terms of ϑ and $1 + \frac{\vartheta}{\Delta}$. Because, for pure superconductor $\vartheta = 0$ as a result, $\Delta = 2\hbar\omega \exp(-\frac{1}{\lambda})$.

3.1.2 The Superconducting Critical Temperature

For equation (3.47) at $T = T_c$, $\Delta = 0$, and $\vartheta = 0$ as a result the equation can be written into two integral terms in order to account for the two parameters.

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega} d\xi \frac{\Delta}{\sqrt{\xi_k^2 + (\Delta+\vartheta)^2}} \tanh\frac{1}{2K_B T_c}\sqrt{\xi_k^2 + (\Delta+\vartheta)^2} + \int_0^{\hbar\omega} d\xi \frac{\vartheta}{\sqrt{\xi_k^2 + (\Delta+\vartheta)^2}} \tanh\frac{1}{2K_B T_c}\sqrt{\xi_k^2 + (\Delta+\vartheta)^2} \tag{3.52}$$

Factorizing out Δ and multiplying both sides of equation (3.52) by $\frac{1}{\Delta}$ it gives:

$$\frac{1}{\lambda} = \int_0^{\hbar\omega} d\xi \frac{1}{\sqrt{\xi_k^2 + (\Delta+\vartheta)^2}} \tanh\frac{1}{2K_B T_c}\sqrt{\xi_k^2 + (\Delta+\vartheta)^2} + \int_0^{\hbar\omega} d\xi \frac{\vartheta}{\Delta\sqrt{\xi_k^2 + (\Delta+\vartheta)^2}} \tanh\frac{1}{2K_B T_c}\sqrt{\xi_k^2 + (\Delta+\vartheta)^2} \tag{3.53}$$

We can find the result of the two integrals of equation (3.53) in order to handle the calculation easily. To find the first integral I_1 we take $E = \sqrt{\xi_k^2 + (\Delta+\vartheta)^2}$.

$$I_1 = \int_0^{\hbar\omega} dE \frac{1}{E} \tanh\frac{E}{2K_B T_c} \tag{3.54}$$

Let, $x = \frac{E}{2K_B T_c}$ which is $dx = \frac{dE}{2K_B T_c}$, and modification of limit of integration should be; $x = \frac{\hbar\omega}{2K_B T_c}$ is the upper limit and $x = 0$ is the lower limit. Thus; equation (3.54) would likely be evaluated as:

$$I_1 = \int_0^{\frac{\hbar\omega}{2K_B T_c}} dx\, 2K_B T_c \frac{1}{x 2K_B T_c} \tanh x = \int_0^{\frac{\hbar\omega}{2K_B T_c}} \frac{\tanh x}{x} dx \tag{3.55}$$

The last term of equation (3.55) should be expressible as two terms; the first one is exactly evaluated, but the second one can approximated as long as $\frac{\hbar\omega}{2K_BT_c} >> 1$ it's upper limit is to infinity.

$$\int_0^{\frac{\hbar\omega}{2K_BT_c}} \frac{\tanh x}{x}dx = \ln\frac{\hbar\omega}{2K_B\,T_c} - \int_0^{\infty} \frac{\ln(x)}{\cosh^2(x)}dx$$

Immediately equation (3.55) would resulted out the following.

$$I_1 = \ln\frac{4e^{\gamma}}{\pi}\frac{\hbar\omega}{2K_B\,T_c} = \ln 1.13\frac{\hbar\omega}{K_B\,T_c} \tag{3.56}$$

Where, $\gamma = 0.57721$ which is Euler's constant. To calculate the second integral of equation (3.53) we can apply the L'Hopital' rule. Let:

$$f(\Delta) = \vartheta\tanh\frac{1}{2}K_B\,T_c\sqrt{{}^2_k + (\Delta+\vartheta)^2}$$

and

$$g(\Delta) = \Delta\sqrt{{}^2_k + (\Delta+\vartheta)^2}$$

. Their corresponding derivatives also given by:

$$f'(\Delta) = \frac{\vartheta(\Delta+\vartheta)}{2K_B\,T_c\sqrt{{}^2_k + (\Delta+\vartheta)^2}}\operatorname{sech}^2\frac{1}{2K_B\,T_c}\sqrt{{}^2_k + (\Delta+\vartheta)^2}$$

and

$$g'(\Delta) = \frac{{}^2_k + (\Delta+\vartheta)^2 + \Delta(\Delta+\vartheta)}{\sqrt{{}^2_k + (\Delta+\vartheta)^2}}$$

The value of I_2 would reads:

$$I_2 = \int_0^{\hbar\omega} \frac{\vartheta^2\operatorname{sech}^2\frac{1}{2K_BT_c}\sqrt{{}^2_k + \vartheta^2}}{2K_B\,T_c({}^2_k + \vartheta^2)}d \tag{3.57}$$

Taking the relation $\operatorname{sech}^2x = 1 - \tanh^2x$ equation (3.57)becomes:

$$I_2 = \int_0^{\hbar\omega} \frac{\vartheta^2}{2K_B\,T_c({}^2_k + \vartheta^2)}d - \int_0^{\hbar\omega} \frac{\vartheta^2}{2K_B\,T_c({}^2_k + \vartheta^2)}\tanh^2\frac{1}{2K_B\,T_c}\sqrt{{}^2_k + \vartheta^2}d \tag{3.58}$$

In equation (3.58) the first part of the right hand term was neglected because it is very small compared to the second one. As a result I_2 is reduced to the following.

$$I_2 = -\frac{\vartheta}{4K_B T_c} \ln(\frac{\vartheta + \hbar\omega}{\vartheta - \hbar\omega}) \tag{3.59}$$

Inserting the values of equations (3.56) and (3.59) into equation (3.53) and rearranging gives:

$$\ln 1.13 \frac{\hbar\omega}{K_B T_c} = \frac{1}{\lambda} + \frac{\vartheta}{4K_B T_c} \ln(\frac{\vartheta + \hbar\omega}{\vartheta - \hbar\omega}) \tag{3.60}$$

Let's assign $b = \frac{\vartheta}{4K_B T_c} \ln(\frac{\vartheta + \hbar\omega}{\vartheta - \hbar\omega})$ from which we can write an equation to calculate the critical temperature.

$$T_c = \frac{1.13\hbar\omega}{K_B} e^{-(\frac{1}{\lambda} + b)} \tag{3.61}$$

In case of pure superconductor $\vartheta = 0$, this shows that the last term of equation (3.60) reduced to zero. Finally, the critical temperature $T_c = \frac{1.13\hbar\omega}{K_B} e^{-\frac{1}{\lambda}}$ should be in agreement with the fundamental BCS value.

The magnetic order parameter was involved both in equations (3.51) and (3.60) that resulted from the AF spin fluctuation property of LiF eAs superconductor. In order to incorporate the spin fluctuation effects on Δ and T_c, we should have to apply McMillan's equation, because this equation is a powerful to approximate the superconducting properties of materials[51,53]. Thus; the McMillan's equation used to estimate Δ and T_c in case of AF spin fluctuation would likely be written as follow:

$$\Delta = \frac{\omega_{ph}}{1.45} \exp(-\frac{1.04(1 + \lambda_{ph} + \lambda_{sf})}{\lambda_{sf} - \lambda_{ph} - \mu^*[1 + 0.62(\lambda_{ph} + \lambda_{sf})]}) \tag{3.62}$$

$$T_c = \frac{\theta_D}{1.45} \exp(-\frac{1.04(1 + \lambda_{ph} + \lambda_{sf})}{\lambda_{sf} - \lambda_{ph} - \mu^*[1 + 0.62(\lambda_{ph} + \lambda_{sf})]}) \tag{3.63}$$

Where; λ_{ph} and λ_{sf} are phonon and spin fluctuation coupling constants respectively satisfying that $1.5 < \lambda_{tot} < 2.99$ ($\lambda_{tot} = \lambda_{ph} + \lambda_{sf}$) and μ^* is Coulomb pseudopotential of the compound[2]. $\theta_D = \frac{\hbar\omega}{K_B}$, which is Debye temperature, whereas ω_{ph} is phonon frequency that is expressible in the order of Debye energy[53].

Chapter 4

Results and Discussion

4.1 Results

By using the model Hamiltonian formulated in chapter 3, the EOM was derived through involving retarded Green's Function. Based on the EOM, we obtain the expressions for the superconducting energy gap at zero temperature $\Delta(0)$ and the superconducting transition temperature T_c of the compound. Since the magnetic property of LiF eAs is AF spin fluctuation, both $\Delta(0)$ and T_c are involving the magnetic order parameter ϑ. If for pure superconductor when the magnetic order parameter is zero, the temperature and the energy gap were reduced to the BCS formalism. But to determine the superconducting energy gap and transition temperature of LiF eAs which are incorporating the magnetic order parameter, we took the estimated values of constants. Accordingly; λ_{ph} can be estimated from the experimental value of T_c so that it should be 0.4[51]. The AF spin fluctuation coupling constant of LiF eAs was 1.9, and we took the approximated value of μ^* to be 0.1[52].

By applying equation (3.62) ($\Delta = \frac{\omega_{ph}}{1.45}\exp(-\frac{1.04(1+\lambda_{ph}+\lambda_{sf})}{\lambda_{sf}-\lambda_{ph}-\mu^*[1+0.62(\lambda_{ph}+\lambda_{sf})]})$), the value of superconducting energy gap has been calculated and approximated to be 4.5mev. Correspondingly, the transition temperature of LiF eAs would be calculated using equation (3.63) ($T_c = \frac{\theta_D}{1.45}\exp(-\frac{1.04(1+\lambda_{ph}+\lambda_{sf})}{\lambda_{sf}-\lambda_{ph}-\mu^*[1+0.62(\lambda_{ph}+\lambda_{sf})]})$) and it resulted 17.37K. Where the values of phonon frequency and Debye temperature were taken to be 100mev and 386K respectively[43,66]. To show the relationship between the superconducting energy gap and the transition temperature of LiF eAs, theoretically calculated values and standard values have been taken into consideration. To do so, we have used equation (2.8) to plot the superconducting energy gap versus temperature.

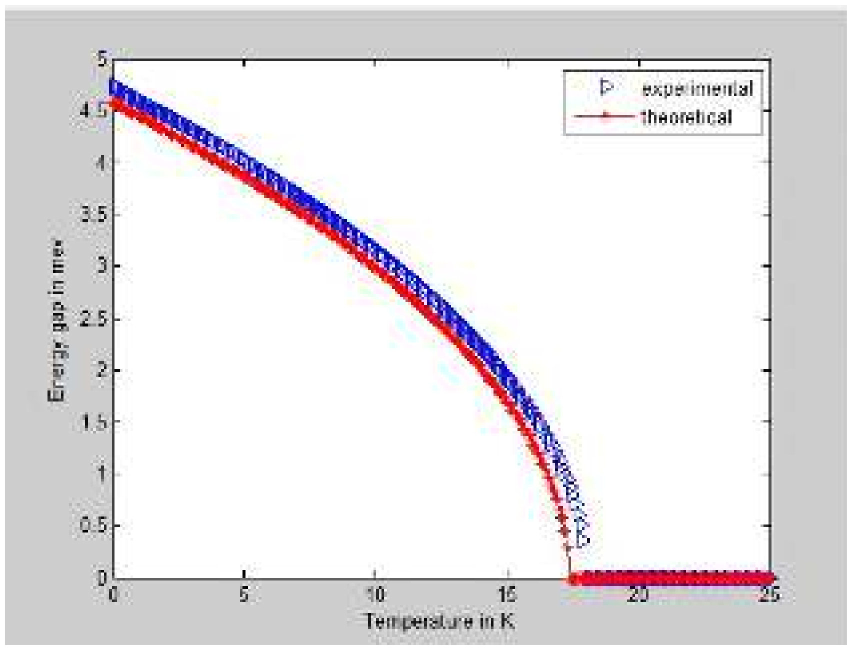

Figure 4.1: Temperature dependence of superconducting energy. The calculated superconducting energy gap versus catculated temperature(red), and experimental superconducting energy gap versus experimental value of temperature(blue).

The theoretical calculated values of both the superconducting energy gap and transition temperature are compared to their experimental values. In Figure 4.1 theoretically calculated value of critical temperature is 17.37K which is less than experimental one, but comparable. In the same way the theoretical value of superconducting energy gap is lower than the typical value.

4.2 Discussion

Two possible mechanisms are responsible for resistivity have been examined in the case of LiF eAs superconductor namely; phonons and AF spin fluctuations. The AF fluctuation behavior of this superconductor was not allowed us to calculate its superconducting parameters straightforward just as BCS theory. In order to treat the spin fluctuation, we have been interested to introduce an interaband coupling that acts only in the first band (incipient band). The BCS theory predicted that both the energy gap and T_c be proportional to the Debye frequency. Importantly the BCS model of coupled electron pairing is recognized with out any reference to the physical origin of the attractive interaction. In addition, there are two reasons why the BCS results are not in a complete agreement with measurements[26]:

1. the interaction between electrons mediated by phonon is retarded in time
2. the damping of quasi-particle states

Thus; due to these reasons the superconductor that we concern could not be analyzed only using the original BCS theory. It needs the extension of this theory to calculate the superconducting transition temperature and energy gap. In this case phonon mediated attractive interaction and the AF fluctuation have taken into consideration to analyze the parameters of LiF eAs superconductor. If the spin-fluctuations are really strong in LiF eAs, they can help to increase the T_c either indirectly, contributing to the DOS renormalization, or providing another, non-phonon mechanism for the superconducting pairing[67]. Accordingly our result was determined based on this concept and come into comparison with the experimental values. We can see that the value of critical temperature is comparable to the experimental value. Even-though the AF fluctuation property of LiF eAs, but due to existence of incipient band one can increase the superconducting strength of this compound.

In general, when the extremum of a band is below the Fermi level but still within the cutoff[14];(where pairing is driven by interaction with incipient band) most work in the literature has addressed this mechanism and prematurely concluded that weak-coupling theories cannot be applied to certain family of FeSCs where evidence for robust pairing was found in the incipient bands.

Chapter 5

Conclusion

We have investigated pairing on a band away from the Fermi level,but not crossing the Fermi level along with phonon mediated interaction. This have been accompanied by presenting a model to study how the phonon driven mechanism supports the spin fluctuation mechanism. The anti-ferromagnetic fluctuation mechanism was handled using the suitable model Hamiltonian in order to harmonize this fluctuation with localized and free electrons to account for superconductivity of LiF eAs. We have tried to show that superconductivity is possible due to incipient band if the system is well established and for-mulating a suitable model Hamiltonian which accounts for derivation of EOM through retarded Green's Function. Based on the EOM, the superconducting energy gap and transition temperature of the superconductor due to incipi-ent have been determined. Finally we recommend that extension of the BCS theory is appreciable without ignoring it's originality to increase the transition temperature of superconductors. We also recommend that understanding the role of incipient band can led for improving transition temperature of certain FeSCs.

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