POSSIBLE MECHANISM OF SUPERCONDUCTIVITY IN Fe-BASED SUPERCONDUCTORS

By

TESFAYE CHEBELEW

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The undersigned hereby certify that they have read and recommend to the School of Graduate Studies for acceptance a thesis entitled "**Possible Mechanism of Superconductivity in Fe-based Superconductors**" by **Tesfaye Chebelew** in partial fulfillment of the requirements for the degree of Master of Science in Physics.

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Prof. P. Singh, Advisor: ____________________

Prof. V. N. Mal'nev, Examiner: ____________________

Dr. Chernet Amente, Examiner: ____________________

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Author: **TESFAYE CHEBELEW**

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Signature of Author

Table of Contents

List of Tables

List of Figures

Abstract

Recent discovery of superconductivity in the Iron-based layered pnictides with transition temperature T_c ranging between 26 and 56K has generated enormous interest in the study of these superconductors. In Iron-based superconductors (Iron-based layered pnictides), superconductivity occurs on doping of either electrons or holes in the FeAs layers. The Iron Fe^{2+}, forms tetrahedron with in the layers. This means that pnictides Fermi level is formed by $3d_{xy}$, $3d_{yz}$, or $3d_{zx}$ orbitals. Very intriguing property of theses new compounds is the rather high flexibility concerning elemental substitution, leading to several families of superconductors, termed '1111', '122','11' and so on, depending on the chemical composition. In this newly discovered Iron-based layered pnictides like cuprates, has triggered challenge towards understanding the pairing mechanism.

In this work we analyze superconductivity of Iron-based superconductor. After reviewing the current finding on this systems, we suggest phonon-exciton combined mechanism to give a right order of supercoducting transition temperature T_c's for whole class of Fe based superconductors.

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Chapter 1

Introduction

The phenomenon of superconductivity, in which the electrical resistance of certain materials completely vanishes at low temperatures, is one of the most interesting and sophisticated in condensed matter physics [5].

The former was due to Kamerlingh Onnes (Kamerlingh Onnes, 1911) who discovered that the electrical resistance of various metals, e. g. mercury, lead, tin and many others, disappeared when the temperature was lowered below some critical value T_c . The actual values of T_c varied with the metal. Subsequently perfect diamagnetism in superconductors was discovered (Meissner and Ochsenfeld, 1933). This property not only implies that magnetic fields are excluded from superconductors, but also that any field originally present in the metal is expelled from it when lowering the temperature below its critical value [35] . These two features were captured in the equations proposed by the brothers F. and H. London (London and London, 1935) who first realized the quantum character of the phenomenon [36].

The decade starting in 1950 was the stage of two major theoretical breakthroughs. First, Ginzburg and Landau (GL) created a theory describing the transition between the superconducting and the normal phases (Ginzburg and Landau, 1950) [34,42]. Seven years later Bardeen, Cooper and Schrieffer (BCS) created the microscopic theory that bears their name (Bardeen et al., 1957). Their theory was based on the fundamental theorem (Cooper, 1956), which states that, for a system of many electrons at low temperature T , any weak attraction, no matter how small it is, can bind two electrons together, forming the so called Cooper pair [36]. In a sense, the Ginzburg and Landau(GL) theory was the prototype of the modern effective theories. Another remarkable advance in these years was the Abrikosovs theory of the type II superconductors (Abrikosov, 1957), a class of superconductors allowing a penetration of the magnetic field, within certain critical values [34].

In 1933, Meissner and Ochsenfeld made another fundamental discovery. They found that superconductors expelled magnetic flux when they were cooled below the transition temperature. This established that there was more to the superconducting state than perfect conductivity (which would require E = 0); it is also a state of perfect diamagnetism or B = 0. For a long, thin superconducting specimen,$B = H + 4\pi M$. Inside superconductors $B = 0$, so $H + 4\pi M = 0$ and $H_{in} = Ba$ (the externally applied B field) by the boundary conditions of H along the length being continuous. Thus,$Ba + 4\pi M = 0$ or $\chi = M/B_a = -1/(4\pi)$, which is the case for a perfect diamagnet. Exclusion of the flux is due to perfect diamagnetism caused by surface currents, which are always induced so as to shield the interior from external magnetic fields. A simple application of Faradays law for a perfect conductor would lead to a constant flux rather than excluded flux [29].

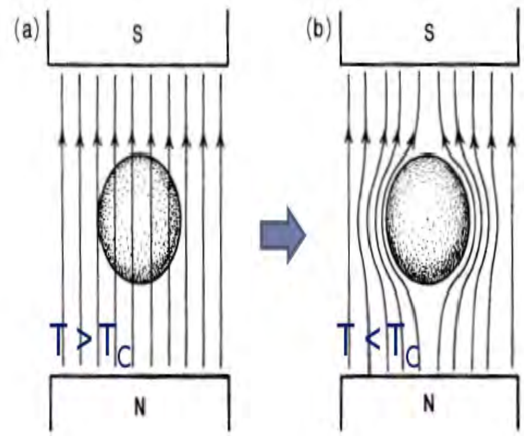

Figure 1.1: The Meissner effect of (a) normal and (b)superconducting states($T>T_c$ and $T<T_c$).

In 1986 Bednorz and Müller reported their discovery of the first of the high- T_c cuprate superconductors (T_c= 30 K) (La-Ba-Cu-O). Since then many investigations have been carried out on the high-T_c superconductors including Y-Ba-Cu-O with $T_c \approx 94$ K. So the potential applications of high-T_c superconductors, which are of type II, appear enormous. The superconducting state of these conductors is essentially the same as that of elemental superconductors [37].

Basic experimental facts, as already said, superconductivity was discovered in 1911 by Kamerlingh Onnes in Leiden (Kamerlingh Onnes, 1911). The basic observation was the disappearance of electrical resistance of various metals (mercury, lead and thin) in a very small range of temperatures around a critical temperature T_c (4.15 K) characteristic of the material (see Fig 1.2) [11].

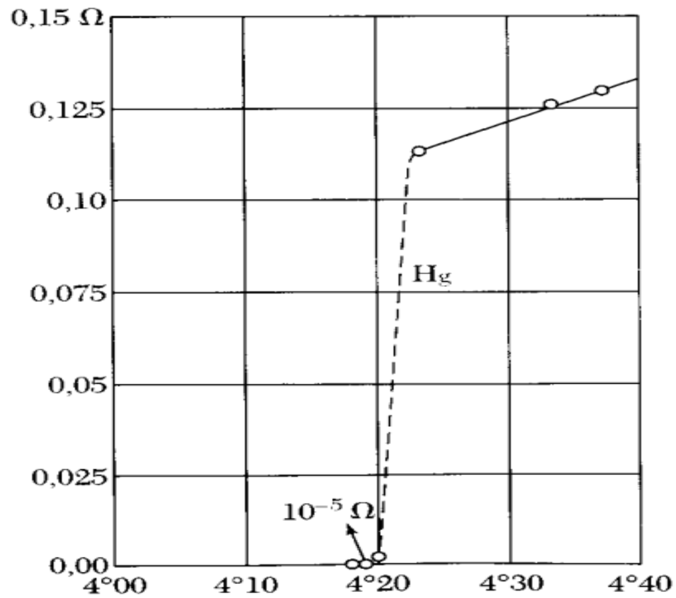

Figure 1.2: Electrical resistance of Mercury Hg at low temperature (Onnes 1913) which showed a transition temperature at 4.2 K.

The spin density wave (SDW) is an antiferromagnetic ground state of metals for which the density of the conduction electron spins is spatially modulated. In conventional antiferromagnets like MnF_2 the magnetic moments have opposite orientation and are located at two crystallographic sublattices. On the contrary the spin-density wave(SDW) is a many-particle phenomenon of an itinerant magnetism which is not fixed to the crystal lattice. Spin-density waves(SDW) are observed in metals and alloys; most prominent is chromium and its alloys. The spin-density wave(SDW) also occurs as ground state in strongly anisotropic systems, for example the one-dimensional organic conductors.Spin-density wave(SDW) is very close to charge-density wave(CDW) since the spin-density $\rho(r)$ for spin σ is modulated in space;a difference is that in spin-density wave(SDW) the spin-density $\rho_{\uparrow}(r){-}\rho_{\downarrow}(r)$ oscillates in space with the charge-density $\rho_{\uparrow}(r){+}\rho_{\downarrow}(r)$ unmodulated,while in charge-density wave(CDW) the charge-density oscillates no net spin-density. The spin-density wave(SDW) state is a kind of antiferromagnrtic state with the electronic, spin density forming a static wave [16].

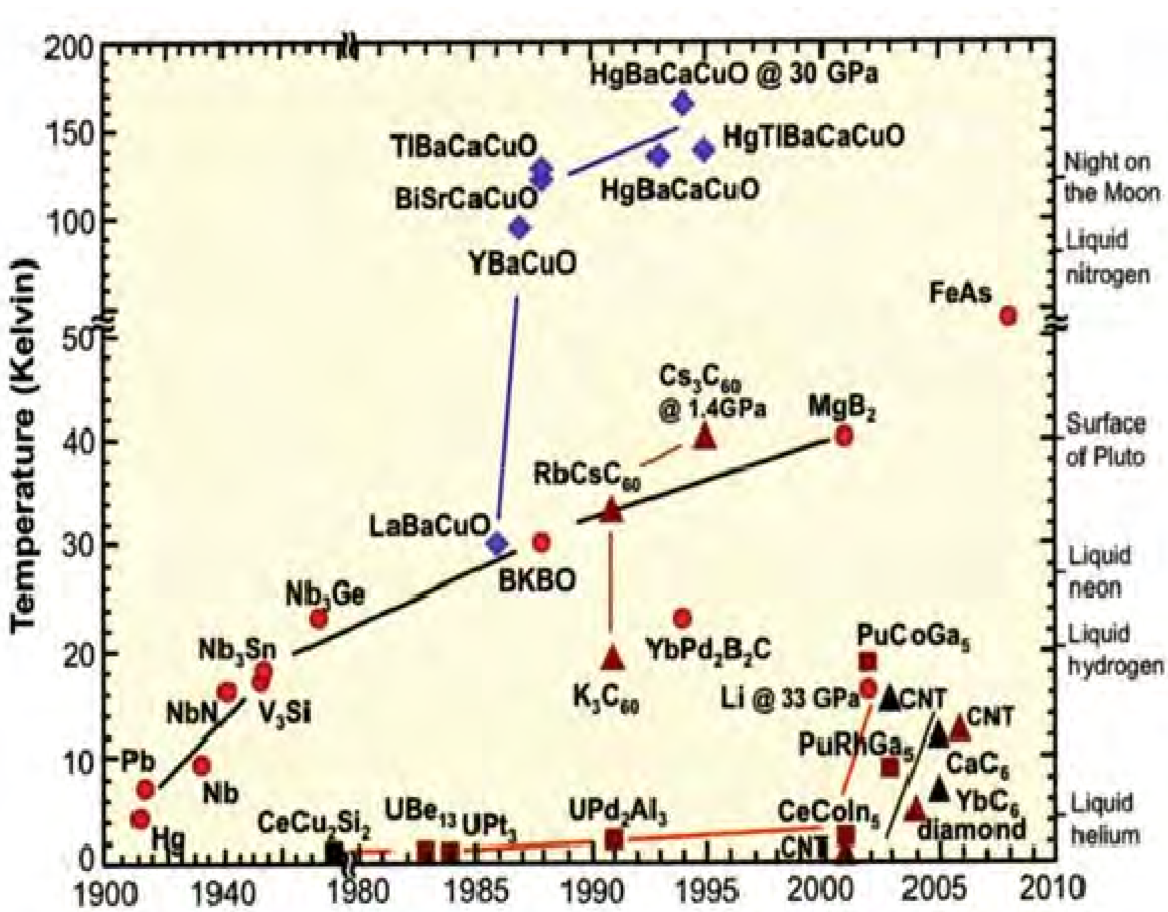

Figure 1.3: The evolution of T_c according to the year of discovery of superconductors.

In 2008, led by recently discovered iron-pnictide compounds (originally known as oxypnictides), they were in the first stages of experimentation and implementation. (Previously most high-temperature superconductors were cuprates and being based on layers of copper and oxygen sandwiched between other substances. These type of superconductors are known as Mott insulators [38].

The discovery of the ferropnictide superconductors have generated tremendous interest in the scientific community because of their high transition temperature and potential for applications. One of the central questions surrounding these materials is the nature of the superconductivity and whether or not it is connected to the antiferromagnetism present in this family of compounds(LaFePO), which was also discovered by (Kamihara et al , 2006), was the first 1111 compound to show superconductivity, but with very low $T_c(\sim 5-7K)$

[8,39]. There is compelling evidence to suggest that the ferropnictides have properties similar to a number of strongly correlated electron materials in which unconventional superconductivity emerges in proximity to antiferromagnetic ground states. Yet there are a number of important distinctions, foremost of which is that the antiferromagnetic parent state of the ferropnictides is an itinerant spin density wave, whereas that of the cuprates is Mott insulating. It is not clear whether the magnetic excitations of these two very different states could be responsible for superconductivity, or whether an unidentified novel pairing mechanism is at play in the Fe-based superconductors(ferropnictides). Therefore, it is crucial to characterize the ordered antiferromagnetic state of the ferropnictides to fully understand the nature of the excitations of the parent material. Fe-based superconductors(ferropnictides) differ from cuprates in terms of their electronic structure, magnetic order, correlation effects, and superconducting symmetry.

For this reason we include literature review of superconductivity, and iron based superconductors(pnictides) in chapter two , mathematical method in chapter three, theoretical Formulation(formulation of the problem) in chapter four and in the last chapter we include results and discussion.

Chapter 2

Review Literature

2.1 Superconductivity

As we mentioned in introduction superconductivity was discovered by Kamelingh Onnes in 1911. He noticed that the resistance of Mercury suddenly drops to the zero at 4.2K. Soon after this discovery, many other elementary metals,compounds and alloy were found to exhibit zero resistance when their temperatures were lowered below a certain characteristic temperature of the material, called the critical temperature, T_c [42].

Element	$T_c(K)$	Element	$T_c(K)$	Element	$T_c(K)$
Al	1.19	Nb	9.2	Tc	7.8
Be	0.026	Np	0.075	Th	1.37
Cd	0.55	Os	0.65	Ti	0.39
Ga	1.09	Pa	1.3	Tl	2.39
Hf	0.13	Pb	7.2	U	0.2
Hg	4.15	Re	1.7	V	5.3
In	3.40	Rh	0.0003	W	0.012
Ir	0.14	Ru	0.5	Zn	0.9
La	4.8	Sn	3.75	Zr	0.55
Mo	0.92	Ta	4.39		
Compound	T_c(K)	Compound	T_c(K)	Compound	T_c(K)
Nb_3Sn	18.1	MgB_2	39	UPt_3	0.5
Nb_3Ge	23.1	$PbMo_6S_8$	15	UPd_2Al_3	2
Cs_3C_{60}	19	YPd_2B_2c	23	$(TMTSF)_2CIO_4$	1.2
Cs_3C_{60}	40	$HoNi_2B_2C$	7.5	$(ET)_2Cu[Ni(CN)_2]Br$	11.5

Table 2.1: The critical temperatures of some superconductors.

High-T_c superconductor	T_c(K)	High-T_c superconductor	T_c(K)
$La_{1.83}Sr_{0.17}CuO_4$	38	$TlBa_2Ca_2Cu_3O_{10+x}$	125
$YBa_2Cu_3O_{6+x}$	93	$HgBa_2Ca_2Cu_3O_{8+x}$	135
$Bi_2Sr_2Ca_2Cu_3O_{10+x}$	107	$Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.33}$	134
		$Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.33}$	155

Table 2.2: High-T_c superconductors.

Supercoductivity occurs when electrical resistivity of specimen drops to zero jump bellow the critical (transition) temperature,T_c. Below critical temperature,T_c resistivity is zero,not just close to zero.At low-temperature resistivity of a normal metals can be written as [5,27]

$$\rho_{(T)}=\rho_o+BT^5 \quad (2.1.1)$$

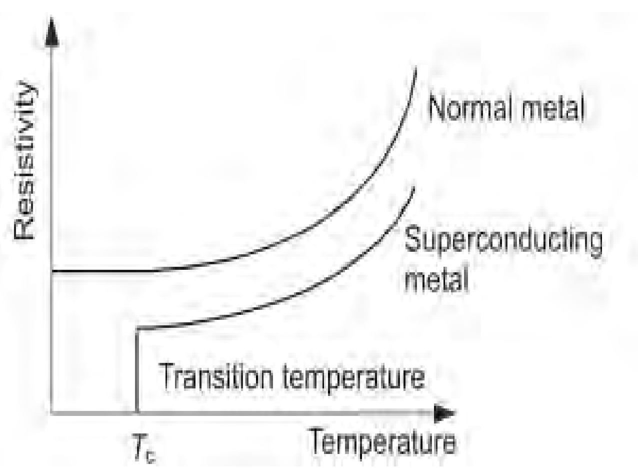

Figure 2.1: Electrical resistivity in normal and superconducting metals (schematic) [29].

containing nonmagnetic impurities.

2.1.1 Magnetic susceptibility of superconductors

Walter Meissner and Robert Ochsenfeld (in 1933) were discovered a magnetic phenomenon that showed that superconductors are not just perfect conductors. Imagine that both the ideal conductor and superconductor are above their critical temperature, T_c . That is, they both are in a normal conducting state and have electrical resistance ($T > T_c$). A magnetic field, B_a, is then applied. This results in the field penetrating both materials. Both samples are then cooled so that the ideal conductor now has zero resistance. It is found that the superconductor expels the magnetic field from inside it, while the ideal conductor maintains its interior field. According to Lenz's law a current would be generated, which would oppose the flux, and eject any magnetic field from the superconductors. For the case, when magnetic field is expelled from superconductor, we can write [5,11].

$$B = \mu_o (H + M) = \mu_o H (1 + \chi) \tag{2.1.2}$$

Where M is magnetization,χ is magnetic susceptibility and H is magnetic field. If B=0 for the case superconductor. From the eq(2.1.2)

$$\chi = -1 \tag{2.1.3}$$

These show that superconductors are perfect diamagnets.

2.1.2 Meissner effect in high-T_c superconductors

Common demonstration of the Meissner effect is to cool a high-T_c superconductor ($YBa_2Cu_3O_7$), then place a small and strong permanent magnet on top of it to demonstrate the repulsion of the magnetic field by the superconductor(see fig 2.2). This repulsion results in the levitation of the magnet. An explanation for this levitation is that the magnet sees a mirror image of itself in the superconductor, which is like a magnet floating on top of another identical magnet. This would be true if the superconductor was much larger than the magnet. In practice the superconductor may be only slightly larger than the magnet. This will result in a distorted image of the magnet, especially near the edges of the superconductor. The situation then is similar to trying to balance two magnets on top of each other [5].

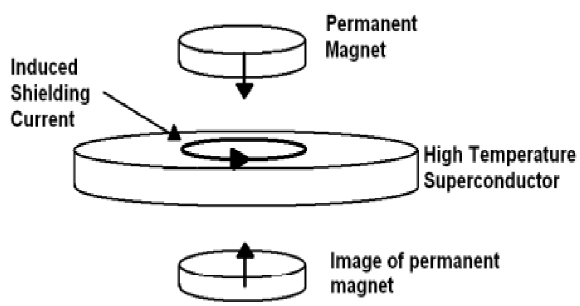

Figure 2.2: Levitating permanent magnet on top of a high- T_c superconductor.

2.1.3 Critical magnetic field and Critical current

The superconducting state can be destroyed not only increasing the temperature but also by applying a magnetic field H(H.K onnes, 1914). If T_c is the critical temperature at zero magnetic field, then the experimental dependence of the critical field H_c on T is

$$H_c(T) = H_c\left[1 - \left(\frac{T}{T_c}\right)^2\right], T \leq T_c \tag{2.1.4}$$

i.e the critical magnetic field is reduced to zero at T_c, here H_c is critical magnetic at zero temperature.

From the above the critical temperature in a nonzero magnetic field is actually different from T_c at zero field. i.e the critical temperature

$$T_c(H) = T_c\sqrt{1 - \frac{H}{H_c(0)}} \tag{2.1.5}$$

is shifted downwards by the applied field, reaching at $H=H_c$

Superconductivity can also be destroyed by strong electric currents.The empirical law (F.B. Silsbee,1916) is that the critical current creates a magnetic field equal to H_c at the surface of the superconducting sample [23].

Year	Scientists	Contribution
1913	H. K. Onnes	Properties of materials at low temperature
1972	J.Bardeen, L.Cooper,and R.Schrieffer	Microscopic(BCS) theory of conventional superconductors
1973	I.Giaever and B.Josephson	Tunnelling effect in superconductors
1986	J.G.Bednorz and K.A Muller	Discovery of the copper oxide-based high temperature supeconductors
1991	P.de Gennes	Studies on complex systems including superconductivity
2003	V.L Ginzburg and A.A Abrikosov	For pioneering contributions to the theory of superconductors

Table 2.3: Nobel price in Physics for contribution to superconductivity [21].

2.1.4 Type of superconductors

Type-I superconductors are superconductors that cannot be penetrated by magnetic flux lines (complete Meissner effect). As such, they have only a single critical temperature at which the material ceases to superconduct, becoming resistive. Elementary metals, such as aluminum, mercury and lead behave as typical Type I superconductors below their respective critical temperatures.

But,Type-II superconductor is a superconductor characterized by its gradual transition from the superconducting to the normal state within an increasing magnetic field. Typically they superconduct at higher temperatures and magnetic fields than Type-I superconductors. This allows them to conduct higher currents. Type-II superconductors are usually made of metal alloys or complex oxide ceramics [28].

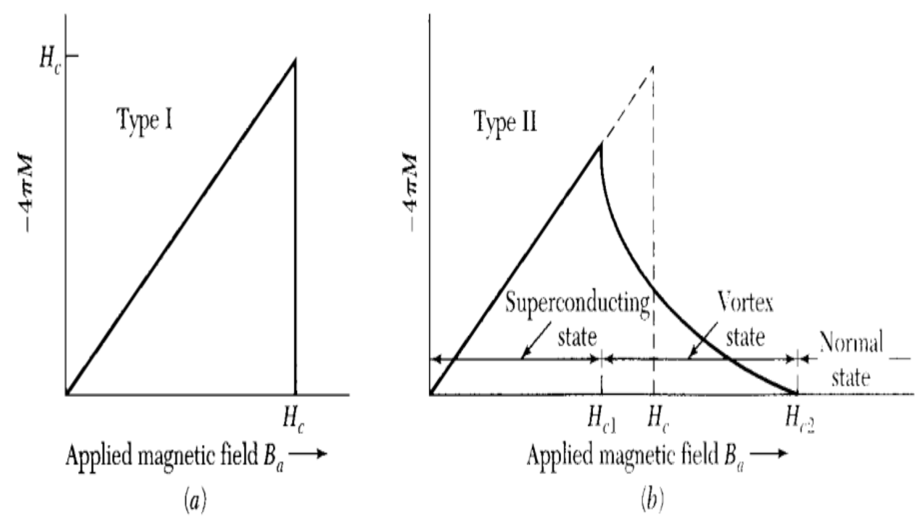

Figure 2.3: Graphic represantation of (a) type- I and type-II superconductors

2.1.5 London equation

London equation can correctly predict magnetic field penetration into the superconducting (SC) material, but cannot give a microscopic picture. Let assume a two fluid model where we distinguish between normal and superconducting (SC) electrons.

$$n{=}n_n{+}n_S \tag{2.1.6}$$

Where n is density of electron, n_n is density of normal state and n_S is density of superconducting (SC) state.

For superconducting electrons in electronic field we can write

$$m\frac{dV_s}{dt} = -eE \tag{2.1.7}$$

If we consider equation for current density and apply it for superconducting (SC) electron.

$$j_s = -en_sV_s \tag{2.1.8}$$

We get

$$\frac{dj_s}{dt} = \frac{n_se^2}{m}E \tag{2.1.9}$$

combining this with Faraday's law

$$\nabla \times E = -\frac{\partial B}{\partial t} \tag{2.1.10}$$

We obtain

$$\frac{\partial\left(\nabla \times E + \frac{n_se^2B}{m}\right)}{\partial t} = 0 \tag{2.1.11}$$

$$\nabla \times j_s = -\frac{n_se^2}{m}B \tag{2.1.12}$$

$$\nabla \times B = \mu_o j_s \tag{2.1.13}$$

we get

$$\nabla^2 B = \frac{\mu_o n_s e^2}{m}B = \frac{1}{\lambda^2}B \tag{2.1.14}$$

Where

$\lambda = \left(\frac{m}{\mu_o n_s e^2}\right)^{1/2}$ is a London penetration depth, which measures the penetration of the magnetic field.

$$B(x) = B_o e^{-x/\lambda} \tag{2.1.15}$$

This equations in turn, predicts currents and magnetic field in superconductors can exist only within a layer of thickness λ of the surface and magnetic field decay in superconductor exponentially; where λ is known as the london penetration depth [7].

2.1.6 BCS theory (Bardeen, Cooper and Schrieffer)

Bardeen, Cooper and Schrieffer also describe superconductivity as a microscopic effect caused by Bose-Einstein condensation of pairs of electrons (Cooper pairs) in the presence of an attractive potential. The pairs with opposite spins act like bosons and leave an energy gap $\varDelta$ (a few meV) between the BCS ground state and the first excited state.

$$\Delta(0K) = 2\hbar\omega_D exp\left(-\frac{1}{V_o N_{E_f}}\right) \tag{2.1.16}$$

ω_D is Debye frequency, V_o is coupling potential and N_{E_f} is density of states of single-electron at the Fermi energy.

The energy gap inhibits a kind of collision interaction (resistivity), if the transfer energy by the collision is smaller than the gap. The critical temperature T_c for superconductivity is a measure of the energy gap [6].

$$T_c = 1.14\frac{\hbar\omega_D}{K_B} exp\left(-\frac{1}{V_o N_{E_f}}\right) \tag{2.1.17}$$

Mc Millan equation [48]

$$T_c = \frac{\theta_D}{1.45} exp[\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}] \tag{2.1.18}$$

Where θ_D is the Debye temperature, μ^* is coulomb pseudo potential and λ is electron-phonon coupling constant.

Bogoliubov model gives

$$T_c \propto \omega_d exp(\frac{-1}{\lambda - \mu}) \tag{2.1.19}$$

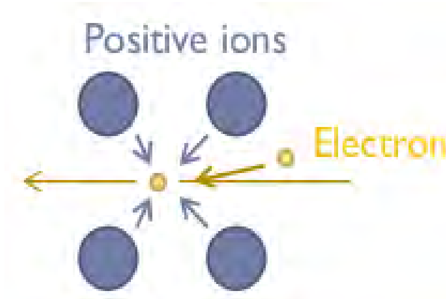

Figure 2.4: A picture of an attractive interaction (phonon interaction).

2.2 Superconductivity in ferropnictides (iron-pnictides)

High-T_c superconductivity at 26 K was reported by Kamihara et al. in F-doped LaFeAsO in a two-pages paper that appeared on line in 23rd of February 2008. This was the discovery of high-Tc superconductivity in a completely new class of materials that came to be known as iron-pnictides. This new discovery has generated a great interest in the materials science community opening a new route for the high-T_c research in addition to that of the cuprates. However, this has also brought new challenges on both experimental and theoretical sides and added a new problem for material scientists in addition to the long- standing problem of cuprates [8,20].

Material	T_c(K)	Material	T_c(K)
$LaO_{1-x}F_xFeAs$	26	$Ba_{1-x}Rb_xFe_2As_2$	23
$NbFeAsO_{1-x}F_x$	52	$K_{1-x}Sr_xFe_2AS_2$	36
$PrFeAsO_{1-x}F_x$	52	$Cs_{1-x}Sr_xFe_2AS_2$	37
$SmFeAsO_{1-x}F_x$	55	$Ca_{1-x}Na_xFe_2As_2$	20
$CeFeAsO_{1-x}F_x$	41	$Eu_{1-x}K_xFe_2As_2$	32
$GdFeAsO_{1-x}F_x$	50	$Eu_{1-x}Na_xFe_2As_2$	35
$TbFeAsO_{1-x}F_x$	46	$Ba(Fe_{1-x}Co_x)_2As_2$	22-24
$DyFeAsO_{1-x}F_x$	45	$Ba(Fe_{1-x}Ni_x)_2As_2$	20
$Gd_{1-x}Th_xFeAsO$	56	$Sr(Fe_{1-x}Ni_x)_2As_2$	10
$LaFeASO_{1-y}$	28	$Ca(Fe_{1-x}Co_x)_2As_2$	17
$NdFeAsO_{1-y}$	53	$Ba(Fe_{1-x}Rh_x)_2As_2$	24
$PrFeAsO_{1-y}$	48	$Ba(Fe_{1-x}Pd_x)_2As_2$	19
$SmFeAsO_{1-y}$	55	$Sr(Fe_{1-x}Rh_x)_2As_2$	22
$GdFeAsO_{1-y}$	53	$Sr(Fe_{1-x}Ir_x)_2As_2$	22
$TbFeAsO_{1-y}$	52	$Sr(Fe_{1-x}Pb_x)_2As_2$	9
$DyFeAsO_{1-y}$	52	$Ba(Fe_{1-x}Ru_x)_2As_2$	21
$LaFe_{1-x}Co_xAsO$	14	$Sr(Fe_{1-x}Ru_x)_2As_2$	13.5
$SmFe_{1-x}Ni_xAsO$	10	LiFeAs	18
$SmFe_{1-x}Co_xAsO$	15	$Na_{1-x}FeAs$	25
$LaFe_{1-x}Ir_xAsO$	12	$Fe_{1-y}Se_xTe_{1-x}$	15
$Ba_{1-x}K_xFe_2As_2$	38		

Table 2.4: Summary of the maximum transition temperatures at ambient pressure for various Fe-based superconductors [49].

2.2.1 Pnictides

Pnictides are a relatively new class of superconductors discovered by group at the Tokyo Institute for Technology led by Yoichi Kamihara. They are named for the pnictogen group, which is any member of the nitrogen group including Phosphorous, Arsenic, etc (figure, 2.5). Pnictides are considered a type-II superconductor and thus produce vortices between Hc1 and Hc2 [9].

Figure 2.5: Group consisting of pnictogens.

2.2.2 1111,122,111 and 11 Ferropnictides Families

1111 family

Following the discovery of high-T_c superconductivity in $LaFeAsO_{1-x}F_x$, T_c rapidly increased by exchanging lanthanum with rare earth ions of smaller atomic radii in LnFeAsO and appropriate carrier doping or creating oxygen deficiencies, until it reached a maximum value of $\sim 56K$ until now in $Gd_{1-x}Th_xFeAsO$. This family LnFeAsO came to be known as 1111 family. Note that LaFePO, also discovered by Kamihara et al. in 2006, was the first 1111 compound to show superconductivity, but with very low T_c ($\sim$ 5-7 K). In addition to $LaFeAsO_{1-x}F_x$, the most remarkable 1111 compounds that show high-Tc superconductivity discovered until now are: $SmFeAsO_{1-x}F_x$ ($T_c \approx$ 43K), $CeFeAsO_{1-x}F_x$ ($T_c \approx$ 41K) and $NdFeAsO_{1-x}F_x$ ($T_c \approx$ 51K) [41,44] .

122 family

M. Rotter et al. proposed $BaFe_2As_2$ as a potential new parent compound based on the similarities between $BaFe_2As_2$ and LaFeAsO. In fact, both compounds contain identical (FeAs) layers, and have the same charge accordance as follows: Ba^{2+} $[(F\ eAs)^-\ ]_2$

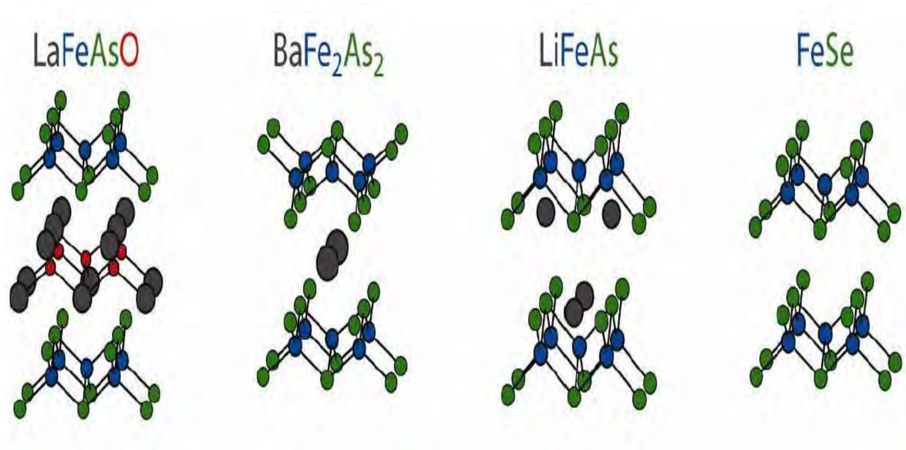

Figure 2.6: Crystal structure of 1111, 122, 111 and 11 respectively.

vs.$(LaO)^+$ $(FeAs)^-$. Partial replacement of Barium with Potassium (hole doping) induced superconductivity at 38 K in $Ba_{0.6}K_{0.4}Fe_2As_2$, the first member of a new family of superconducting iron arsenides known as the 122 family. This discovery was followed by reports of similar compounds with: strontium ($T_c \approx$ 37K), calcium ($T_c \approx$ 20K), and europium ($T_c \approx$ 32K)[39,45].

111 family

X. C. Wang et al. reported the discovery of another new superconducting iron arsenide system LiFeAs (termed 111). Superconductivity with T_c up to 18 K was found in these compounds [8, 46].

11 family

F.C. Hsu et al.reported the observation of superconductivity with zero resistance transition temperature at 8 K in the PbO-type α- FeSe compound known as 11 family. Although FeSe has been studied quite extensively, a key observation is that the clean superconducting phase exists only in those samples prepared with intentional Se deficiency [8,43].

2.2.3 Structure of LaOFeAs

Pnictides are layered, similar to cuprates. The iron-arsenic plane is considered to produce the same effect as the copper-oxygen plane in cuprates and to be responsible for the superconductivity found in pnictides. For example, the critical temperature of LaOFeAs was found to increase with a doping of fluorine. The doping was found to increase the number of carriers in the conductive layer. Figure 2.7, from an article on LaOFFeAs shows the layered structure with the formation of carriers in the conductive layer.

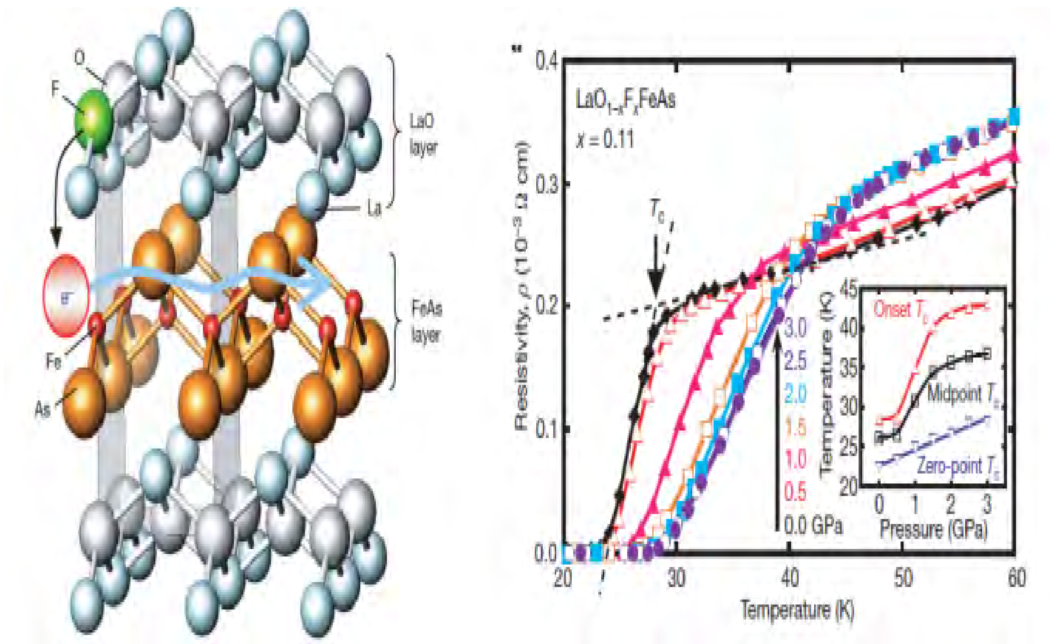

Figure 2.7: (a) LaOFFeAs. Doping of the F in the oxygen spaces causes an increase in the number of electron carriers. (b) Resistivity data for $LaO_{1-x}F_xFeAs$ for different pressures. Note as the pressure increases, the critical temperature appears to increase.

The iron, Fe^{2+}, forms tetrahedrons within the layers. According to the article by Yoichi Kamihara, this means that the pnictides Fermi level is formed by $3d_{xy}$, $3d_{yz}$, or $3d_{zx}$ orbitals. This is markedly different from cuprates, which form a square, planar structure and where there is $3dx^2$-y^2 symmetry [8,31].

2.2.4 Antiferromagnetic order

Since superconductivity in iron-pnictides appears by doping their parent compounds with charge carriers, it is natural to wonder what the ground states of the parent compounds are. Also an anomaly in the resistivity of the parent compounds of these materials occur below a certain temperature (150 K in the case of LaFeAsO) in addition to a small anomaly in the d.c. magnetic susceptibility. Optical conductivity and theoretical calculations suggest that LaFeAsO exhibits a spin-density-wave (SDW) instability that is suppressed by doping with electrons to induce superconductivity.

However, the first direct evidence of SDW order in LaFeAsO came from neutron-scattering experiments by de la Cruz et al. [10]. These experiments demonstrated that LaFeAsO undergoes an abrupt structural distortion below ∼155 K, changing the symmetry from tetragonal (space group P4/nmm) to monoclinic (space group P112/n) at low temperatures, and then, at ∼137 K, develops long-range SDW-type antiferromagnetic (AFM) order with a small moment but simple magnetic structure. The magnetic structure is consistent with theoretical predictions, but the moment of 0.36μB per iron atom observed here at 8 K is much smaller than the predicted value of $\sim 2.3\mu$B per iron atom. Later, the AFM order in $BaFe_2As_2$ was also observed by a neutron diffraction study by Huang et al.[11]. Similar to the case of LaFeAsO, $BaFe_2As_2$ shows a tetragonal-to-orthorhombic distortion structural transition and magnetic transition. However, both transitions occur simultaneously in $BaFe_2As_2$ in contrast with the separated transitions observed previously in LaFeAsO.

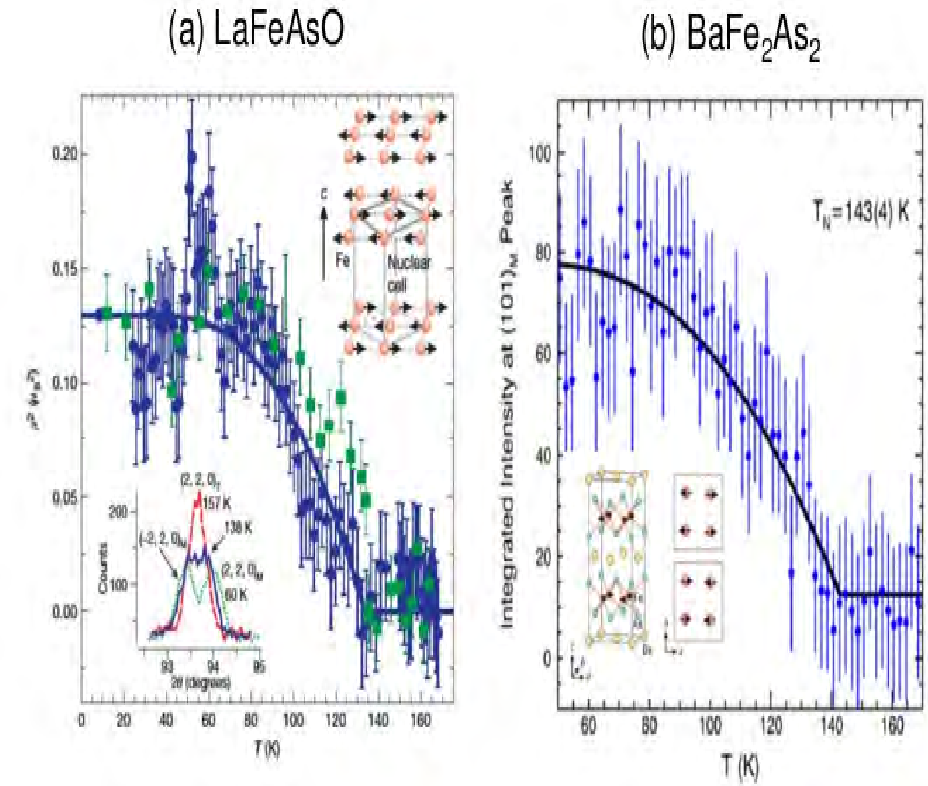

Figure 2.8: Antiferromagnetic ordering in (a) LaFeAsO and (b) $BaFe_2As_2$.

The following table represents the different rare earth matterials shows different transition temperature with fluorine doping and with oxygen deficiency. The Origonal compound is $LaF_xO_{1-x}FeAs$ with T_c=26K. The μSR (muon spin resonance) transport measurement and mössbauer experiment is on the phase diagram of $REO_{1-x}F_xFeAs$ shows the first order like phase transition between antiferromagnetic and superconducting phases [14].

Flourine doped

$CeO_{1-x}F_xFeAs$	41K
$PrO_{1-x}F_xFeAs$	52K
$NdO_{1-x}F_xFeAs$	51K
$SmO_{1-x}F_xFeAs$	43K
$GdO_{1-x}F_xFeAs$	36K

Doping by oxygen deficency

$LaO_{1-x}FeAs$	31K
$SmO_{1-x}FeAs$	55K
$CeO_{1-x}FeAs$	46K
$NdO_{1-x}FeAs$	53K
$PrO_{1-x}FeAs$	51K

Figure 2.9: shows the different rare earth ion superconductors with Transition temperature.

2.2.5 Electronic states

Superconductivity is a manifestation of quantum mechanics on a macroscopic scale. It is important to find whether the superconductivity in the new class of Fe based superconductors is conventional or unconventional like in the cuprates or have an entirely new mechanism. In conventional superconductors, it has been well established that electrons form so called cooper pairs to give rise to the superconductivity. The pair binding manifests itself as an energy gap in many spectroscopic measurements, the energy gap known as superconducting gap, appears at the transition temperature T_c where the resistance also vanishes. For high temperature superconductors this is more complicated since over the wide region of compositions and temperatures this energy gap exists quite well above the transition temperature and there is no relation between transition temperature and this energy gap. This is why this gap is called pseudo gap. The origin of pseudo gap and the relation with the superconducting gap is believed to be the key to understand the mechanism of high temperature superconductivity.

All the conventional superconductors are well understood within the BCS theory as

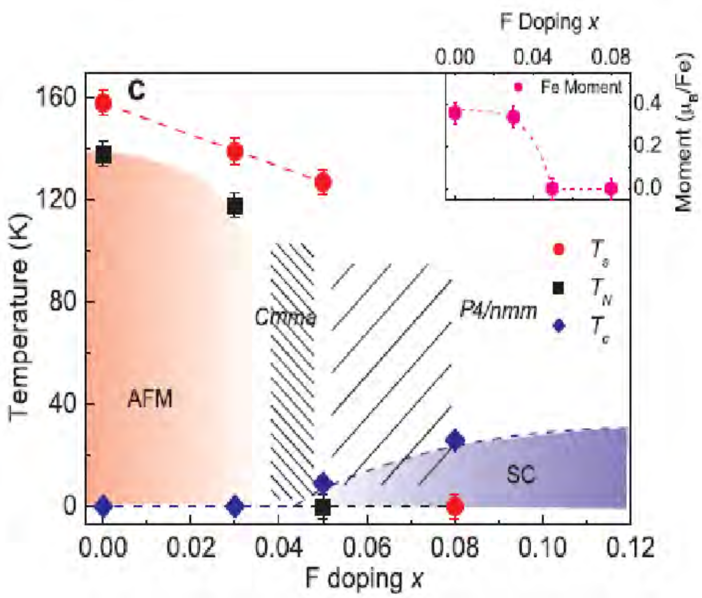

Figure 2.10: Phase diagram determined from neutron measurements on $LaFeAsO_{1-x}F_x$ with x = 0, 0.03, 0.05, 0.08. The red circles indicate the onset temperature of the P4/nmm to Cmma phase transition. The black squares designate the Neel temperatures of Fe as determined from neutron measurements in the inset shows the dependence of the magnetic moment from doping.

phonon mediated pairing of electrons and condensation of the resulting bosonic gas. All superconductors that can be understood within this theory have a transition temperature less than 40K. Preliminary experimental results such as specific heat, NMR spectroscopy and high field resistivity measurement suggest the existence of unconventional superconductivity in these Fe based superconductors [13]. It is pointed out that there is an essential similarity of electronic states near the Fermi level in 122 and 1111 family. Both families have been studied in many details by DFT (density functional theory) calculation. DFT is the quantum mechanical theory used in physics to investigate the electronic structure of many body systems principally the ground state.

2.3 Spin-density wave(SDW)

Spin density wave (SDW) and charge density wave (CDW) are the names for two similar low energy ordered states of solids. Both these states occur at low temperature in anisotropic, low dimensional materials. These both instabilities develop in the presence of Fermi surface nesting. Charge density wave (CDW) couples to the lattice while spin density wave (SDW) couples to the spin.

The spin-density wave(SDW) state is a kind of antiferromagnrtic state with the electronic, spin density forming a static wave. The density varies periodically as a function of the position r with no net magnetization in the entire volume. Specifically, spin-density wave(SDW) occurs with spacial spin-density modulation due to delocalized(or itinerant) electron rather than localized ones.

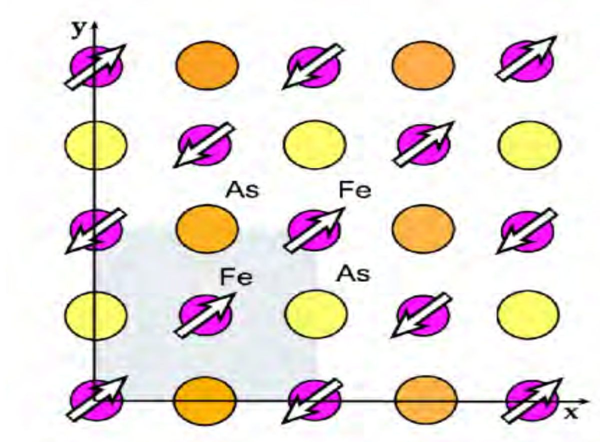

Figure 2.11: The spin-density-wave (SDW) order as observed by the neutron diffraction. The Fe magnetic moments along (1,1) direction are aligned, while the two nearest neighboring Fe are antiferromagnetically aligned.

In the normal state the density $\rho_{\uparrow}(r)$ of electron polarized upward with respect to any quantization axis is completely canceled by the density $\rho_{\downarrow}(r)$ of downward polarized spin. In the spin-density wave(SDW), however the difference $\sigma(r)$ between $\rho_{\uparrow}(r)$ and $\rho_{\downarrow}(r)$ is finite and mundulates in space as a function of the position vector r in spin-density wave(SDW) state [16].

$$\rho_{(r)} = \rho_{\uparrow}(r) - \rho_{\downarrow}(r) \tag{2.3.1}$$

$$\rho_{(r)} = \rho_{\uparrow}(r) + \rho_{\downarrow}(r) \tag{2.3.2}$$

equation (2.3.1) for spin-density wave(SDW) and equation (2.3.2) for charge density wave (CDW).

Chapter 3

Methodology

3.1 Introduction

In this study we have used a quantum field theory of Green's functions technique to obtain the expression for superconducting transition temperature T_c and order parameters (Δ). The Green's functions are useful, because they are flexible enough to describe the effects of retarded interaction and all the quantities of physical interaction can be derived from them. In many-particle physics we adopt the Green's function philosophy and define some simple building blocks, also called Green's functions,from which we obtain solutions to our problems. The Green's functions contain only part of the full information carried by the wave functions of the systems but they include the relevant information for the given problem [24, 26].

3.2 Green functions formalism

Green functions or suitable modification of these functions have been applied in quantum field theory to statistical problem. The Green functions are essentially useful for summing over the restricted classes of perturbation theory diagrams and are very powerful when combined with spectral representations. In quantum field theory Green functions are known as propagator. This name is based on the idea that, in order to find the important physical properties of a systems, it is essential to know, not the detailed behavior of each particle in the system, but rather just the average behavior of one or two typical particles. The quantities that describe this average behaviors are known as the one-particle and two-particle propagation [24].

Green function play the most important part in the field-theoretical treatment of the many-body problem. In our discussion we used only the retarded double-time Green function. It is defined as

$$G(t,t') = \langle\langle \hat{A}(t); \hat{B}(t')\rangle\rangle \tag{3.2.1}$$

$$G(t,t') = -i\theta(t,t')\langle\big[\hat{A}(t), \hat{B}(t')\big]\rangle \tag{3.2.2}$$

Where

$\langle\langle$.................$\rangle\rangle$ is the abbreviated notation for the Green function,

$\langle\langle$............$\rangle\rangle$ denotes the thermal average,

$\theta(t,t')$ is the step function and

$\hat{A}(t)$,$\hat{B}(t')$ are operators in the Heisenberg representation, which can be expressed as the product of the quantized field operator [32].

Then, $A(t) = e^{\left(iHt\right)}A_{(0)}e^{\left(-iHt\right)}$

Also A and B are a commutator or anti-commutator operators. That is

$\big[A, B\big] = AB - BA = 0$ commutator operators and

$\big[A, B\big] = AB - BA \neq 0$ anti-commutator operators.

3.2.1 Equation of motion

There are several ways of attacking the problem, one of which is the equation of motion technique. The basic idea of this method is to generate a series of coupled differential equations by differentiating the Green functions (correlation functions) at hand a number of times.

To obtain the equation of motion of the Green functions we differentiate eq(3.2.2) with respect to time t as

$$\frac{id}{dt}G(t,t') = \delta(t-t')\big\langle\big[\hat{A}(t);\hat{B}(t')\big]\big\rangle - i\theta(t-t')\big\langle\big[i\frac{d}{dt}\hat{A}(t);\hat{B}(t')\big]\big\rangle \tag{3.2.3}$$

$i\hbar\frac{d}{dt}\hat{A}(t) = \big[\hat{A}(t),\hat{H}\big]$

If $\hbar = 1$

$$\frac{id}{dt}G(t-t') = \delta(t-t')\big\langle\big[\hat{A}(t);\hat{B}(t')\big]\big\rangle + \big\langle\big\langle\big[\hat{A}(t),\hat{H}\big],\hat{B}(t')\big\rangle\big\rangle \tag{3.2.4}$$

$\hat{A}(t)$ and $\hat{H}$ satisfy the following condition,

$\big[\hat{A}(t),\hat{H}\big] = \hat{A}(t)\hat{H} - \hat{H}\hat{A}(t)$

Then, equation of motion becomes;

$$\frac{id}{dt}G(t-t') = \delta(t-t')\big\langle\big[\hat{A}(t);\hat{B}(t')\big]\big\rangle + \big\langle\big\langle\hat{A}(t)\hat{H} - \hat{H}\hat{A}(t),\hat{B}(t')\big\rangle\big\rangle \tag{3.2.5}$$

To solve this equation it convenient to work with Fourier transform of this equation. A careful analysis show that the function depends of t and t' through (t-t'). Thus we can write

$G(t,t') = G(t-t')$

Let $G(\omega)$ be the Fourier transform of $G(t-t')$ such that

$$G(t-t') = \int_{-\infty}^{\infty} G(\omega)exp\big(-i\omega(t-t')\big)d\omega \tag{3.2.6}$$

$$G(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G(t-t')exp\big(i\omega(t-t')\big)d(t-t') \tag{3.2.7}$$

and δ function can be defined as

$$\delta(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} exp\big(-i\omega(t-t')\big)d\omega \tag{3.2.8}$$

Therefore eq(3.2.4) becomes

$$\omega G(\omega) = \big\langle\big[\hat{A}(t),\hat{B}(t')\big]\big\rangle + \big\langle\big\langle\big[\hat{A}(t),\hat{H}\big];\hat{B}(t')\big\rangle\big\rangle \tag{3.2.9}$$

Then $\omega G(\omega)$ can be written as

$$\omega\langle\langle A, B\rangle\rangle = \langle[A, B]\rangle + \langle\langle[A, H], B\rangle\rangle \tag{3.2.10}$$

$$\omega\langle\langle A, B\rangle\rangle = \langle[A, B]\rangle + \langle\langle AH - HA, B\rangle\rangle \tag{3.2.11}$$

Since $\langle\langle A, B\rangle\rangle$ denote the Fourier transform of the Green functions involving the operator A and B.

Chapter 4

Theoretical Formulation

4.1 Introduction

In this chapter we try to obtain an expression for T_c and Δ from exclusively phonon-exciton combined mechanism and we calculate T_c, reduced gap $\frac{2\Delta}{K_B T_c}$ and compare the value with the experimental one for Fe-superconductors (ferropnictides).

4.2 Exciton Mechanism

The Hamiltonian for the process involving can be expressed as [1,2]

$$H = H_o + H' \tag{4.2.1}$$

Where

$H_O = \sum_{k\sigma} \epsilon_k a^{\dagger}_{k\sigma} a_{k\sigma} + \sum_j \hbar\omega_{el} b^{\dagger}_j b_j$

$H' = \sum_{k_1 k_2 \sigma_1 \sigma_2 j} B^j \left[a^{\dagger}_{mk_1\sigma_1} a_{nk_2\sigma_2} b_j + hc \right]$

Where

$hc = a^{\dagger}_{nk_2\sigma_2} a_{mk_1\sigma_1} b^{\dagger}_j$

$H' = \sum_{k_1 k_2 \sigma_1 \sigma_2 j} B^j \left[a^{\dagger}_{mk_1\sigma_1} a_{nk_2\sigma_2} b_j - a^{\dagger}_{nk_2\sigma_2} a_{mk_1\sigma_1} b^{\dagger}_j \right]$

H' is very similar in appearance to electron-phonon interaction. ϵ_k is the single particle energy of holes which exist the bands.

$a^{\dagger}_{mk\sigma}(a_{mk\sigma})$ are hole creation(annihilation) operators of layer index m, wave vector K and spin σ. $\hbar\omega_{el}$ is energy of exciton or some electronic excitation. B^j is the coupling constant.

$b^{\dagger}_j$ and b_j denote boson creation and annihilation operators respectively.

The system Hamiltonian can be canonically transformed to [47]

$\hat{H} = e^{-i\tau} H e^{i\tau}$

Expanding the above Hamiltonian using power series

$\hat{H} = H_o + H' + i\big[H_o, \tau\big] + \frac{i}{2}\big[H', \tau\big] + ...$

$H' + i\big[H_o, \tau\big] = 0$

and rearranging the expansion becomes

$$H = H_o + \frac{i}{2}\big[H', \tau\big] \tag{4.2.2}$$

$H_{int} = \frac{1}{2}\big[H', \tau\big]$ [1]

We choose τ in such a way that it's commutator with H_o cancels the term H', that is

$$i\big[H_o, \tau\big] = -H' \tag{4.2.3}$$

let

$\tau = i\sum_{k_1k_2\sigma_1\sigma_2j} B^j\big\{Ca^{\dagger}_{mk_1\sigma_1}a_{nk_2}\sigma_2 b_j - Da^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j\big\}$

C and D are constants

To calculate the value of C and D first we can solve for a $[H_o, \tau]$

$$\big[H_o, \tau\big] = \big[\sum_{k\sigma} \epsilon_k a^{\dagger}_{k\sigma}a_{k\sigma}, \tau\big] + \big[\sum_{j} \hbar\omega_{el} b^{\dagger}_j b_j, \tau\big] \tag{4.2.4}$$

The first term can be evaluated as follow

$\big[\sum_{k\sigma} \epsilon_k a^{\dagger}_{k\sigma}a_{k\sigma}, i\sum_{k_1k_2\sigma_1\sigma_2j} B^j\big\{Ca^{\dagger}_{mk_1\sigma_1}a_{nk_2}\sigma_2 b_j - Da^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j\big\}\big]$

$= i\sum_{kk_1k_2\sigma\sigma_1\sigma_2j} \epsilon_k B^j C\big[a^{\dagger}_{k\sigma}a_{k\sigma}, a^{\dagger}_{mk_1\sigma_1}a_{nk_2}\sigma_2 b_j\big] - i\sum_{kk_1k_2\sigma\sigma_1\sigma_2j} \epsilon_k B^j D\big[a^{\dagger}_{k\sigma}a_{k\sigma}, a^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j\big]$

Using the following conditions

$\big[A, B\big]$=AB-BA for bosons

$\big[A,B\big]$=AB+BA for fermions

and

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

$$\big[\sum_{k\sigma}\epsilon_k a^{\dagger}_{k\sigma}a_{k\sigma}, i\sum_{k_1k_2\sigma_1\sigma_2 j}B^j\big\{Ca^{\dagger}_{mk_1\sigma_1}a_{nk_2}\sigma_2 b_j - Da^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j\big\}\big]$$

$$= i\sum_{kk_1k_2\sigma\sigma_1\sigma_2 j}\epsilon_k B^j C\big\{\big[a^{\dagger}_{k\sigma}a_{k\sigma}, a^{\dagger}_{mk_1\sigma_1}\big]a_{nk_2\sigma_2}b_j + a^{\dagger}_{mk_1\sigma_1}[a^{\dagger}_{k\sigma}a_{k\sigma}, a_{nk_2\sigma_2}b_j]\big\}$$

$$-i\sum_{kk_1k_2\sigma\sigma_1\sigma_2}\epsilon_k B^j D\big\{\big[a^{\dagger}_{k\sigma}a_{k\sigma}, a^{\dagger}_{nk_2\sigma_2}\big]a_{mk_1\sigma_1}b^{\dagger}_j + a^{\dagger}_{nk_2\sigma_2}[a^{\dagger}_{k\sigma}a_{k\sigma}, a_{mk_1\sigma_1}b^{\dagger}_j]\big\}$$

$$\big[\sum_{k\sigma}\epsilon_k a^{\dagger}_{k\sigma}a_{k\sigma}, i\sum_{k_1k_2\sigma_1\sigma_2 j}B^j\Big(Ca^{\dagger}_{mk_1\sigma_1}a_{nk_2}\sigma_2 b_j - Da^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j\Big)\big]$$

$$= i\sum_{kk_1k_2\sigma\sigma_1\sigma_2 j}\epsilon_k B^j C\Big[a^{\dagger}_{k\sigma}\big\{a_{k\sigma}, a^{\dagger}_{mk_1\sigma_1}\big\}a_{nk_2\sigma_2}b_j - a^{\dagger}_{mk_1\sigma_1}\big\{a^{\dagger}_{k\sigma}, a_{nk_2\sigma_2}\big\}a_{k\sigma}b_j\Big]$$

$$-i\sum_{kk_1k_2\sigma\sigma_1\sigma_2 j}\epsilon_k B^j D\Big[a^{\dagger}_{k\sigma}\big\{a_{k\sigma}, a^{\dagger}_{nk_2\sigma_2}\big\}a_{mk_1\sigma_1}b^{\dagger}_j - a^{\dagger}_{nk_2\sigma_2}\big\{a^{\dagger}_{k\sigma}, a_{mk_1\sigma_1}\big\}a_{k\sigma}b^{\dagger}_j\Big]$$

$$= i\sum_{kk_1k_2\sigma\sigma_1\sigma_2 j}\epsilon_k B^j C\big\{a^{\dagger}_{k\sigma}\delta_{kk_1}\delta_{\sigma\sigma_1}a_{nk_2\sigma_2}b_j - a^{\dagger}_{mk_1\sigma_1}\delta_{kk_2}\delta_{\sigma\sigma_2}a_{k\sigma}b_j\big\}$$

$$-i\sum_{kk_1k_2\sigma\sigma_1\sigma_2 j}\epsilon_k B^j D\big\{a^{\dagger}_{k\sigma}\delta_{kk_2}\delta_{\sigma\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j - a^{\dagger}_{nk_2\sigma_2}\delta_{kk_1}\delta_{\sigma\sigma_1}a_{k\sigma}b^{\dagger}_j\big\}$$

If $k=k_1$,$k=k_2$,$\sigma=\sigma_1$ and $\sigma=\sigma_2$

$$\big[\sum_{k\sigma}\epsilon_k a^{\dagger}_{k\sigma}a_{k\sigma}, i\sum_{k_1k_2\sigma_1\sigma_2 j}B^j\Big(Ca^{\dagger}_{mk_1\sigma_1}a_{nk_2}\sigma_2 b_j - Da^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j\Big)\big]$$

$$= i\sum_{kk_1k_2\sigma_1\sigma_2 j}B^j C\left(\epsilon_{k_1}-\epsilon_{k_2}\right)a^{\dagger}_{mk_1\sigma_1}a_{nk_2\sigma_2}b_j$$

$$+i\sum_{kk_1k_2\sigma_1\sigma_2 j}B^j D\left(\epsilon_{k_1}-\epsilon_{k_2}\right)a^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j$$

The second term can be also evaluated

$$\big[\sum_j\hbar\omega_{el}b^{\dagger}_j b_j,\tau\big] = \sum_{k_1k_2\sigma_1\sigma_2 j}\hbar\omega_{el}B^j\big[b^{\dagger}_j b_j, Ca^{\dagger}_{mk_1\sigma_1}a_{nk_2\sigma_2}b_j - Da^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j\big]$$

$$= i\sum_{k_1k_2\sigma_1\sigma_2 j}\hbar\omega_{el}B^j C\big[b^{\dagger}_j b_j, a^{\dagger}_{mk_1\sigma_1}a_{nk_2\sigma_2}b_j\big] - i\sum_{k_1k_2\sigma_1\sigma_2 j}\hbar\omega_{el}B^j D\big[b^{\dagger}_j b_j, a^{\dagger}_{nk_1\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j\big]$$

$$= -i\sum_{k_1k_2\sigma_1\sigma_2 j}\hbar\omega_{el}B^j Ca^{\dagger}_{mk_1\sigma_1}a_{nk_2\sigma_2}\big\{b^{\dagger}_j b_j, b_{j'}\big\} + i\sum_{k_1k_2\sigma_1\sigma_2 j}\hbar\omega_{el}B^j Da^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}\big\{b^{\dagger}_j b_j, b^{\dagger}_{j'}\big\}$$

$$= -i\sum_{k_1k_2\sigma_1\sigma_2 j}\hbar\omega_{el}B^j Ca^{\dagger}_{mk_1\sigma_1}a_{nk_2\sigma_2}b_j\big[b^{\dagger}_j, b_{j'}\big] + i\sum_{k_1k_2\sigma_1\sigma_2 j}\hbar\omega_{el}B^j Da^{\dagger}_{nk_2\sigma_2}a_{mk_1\sigma_1}b^{\dagger}_j\big[b_j, b^{\dagger}_{j'}\big]$$

If $j=j'$

$= -i\sum_{k_1k_2\sigma_1\sigma_2j} \hbar\omega_{el} B^j C a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} b_j + i\sum_{k_1k_2\sigma_1\sigma_2j} \hbar\omega_{el} B^j D a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_j$

Therefore eq(4.2.4) becomes

$$\begin{aligned}\left[H_o,\tau\right] &= i\sum_{k_1k_2\sigma_1\sigma_2j} B^j C\left(\epsilon_{k_1}-\epsilon_{k_2}-\hbar\omega_{el}\right) a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} b_j \\ &+ i\sum_{k_1k_2\sigma_1\sigma_2j} B^j D\left(\epsilon_{k_1}-\epsilon_{k_2}+\hbar\omega_{el}\right) a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_j \end{aligned} \tag{4.2.5}$$

From this we can get the value C and D

$C = \left(\epsilon_{k_1}-\epsilon_{k_2}-\hbar\omega_{el}\right)^{-1}$

and

$D = \left(\epsilon_{k_1}-\epsilon_{k_2}+\hbar\omega_{el}\right)^{-1}$

Therefore

$\tau = i\sum_{k_1k_2\sigma_1\sigma_2j} B^j \left[\frac{a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} b_j}{\epsilon_{k_1}-\epsilon_{k_2}-\hbar\omega_{el}} - \frac{a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_j}{\epsilon_{k_1}-\epsilon_{k_2}+\hbar\omega_{el}}\right]$

To simplify for $\left[H',\tau\right]$ we use similar way

$$\begin{aligned}\left[H',\tau\right] &= i\sum_{k_1k_2\sigma_1\sigma_2j} \left|B^j\right|^2 \left\{ \frac{\left[a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} b_j, a^\dagger_{k_1\sigma_1} a_{nk_2\sigma_2} b_j\right]}{\epsilon_{k_1}-\epsilon_{k_2}-\hbar\omega_{el}} \right. \\ &- \frac{\left[a^\dagger_{mk_1\sigma_1\sigma_1} a_{nk_2\sigma_2} b_j, a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_{j'}\right]}{\epsilon_{k_1}-\epsilon_{k_2}+\hbar\omega_{el}} \\ &- \frac{\left[a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_j, a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} b_{j'}\right]}{\epsilon_{k_1}-\epsilon_{k_2}-\hbar\omega_{el}} \\ &\left. + \frac{\left[a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_j, a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_{j'}\right]}{\epsilon_{k_1}-\epsilon_{k_2}+\hbar\omega_{el}} \right\} \end{aligned} \tag{4.2.6}$$

Since $b^\dagger_j$ and b_j are Boson operators, as a result the first and the last terms is zero.The the second and the third terms can be evaulate as follow

$i\sum_{k_1k_2\sigma_1\sigma_2j} \left|B^j\right|^2 \frac{\left[a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} b_j, a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_{j'}\right]}{\epsilon_{k_1}-\epsilon_{k_2}+\hbar\omega_{el}}$

$= -i\sum_{k_1k_2\sigma_1\sigma_2j} \left|B^j\right|^2 \frac{a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} \left\{a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} b_j, b^\dagger_{j'}\right\}}{\epsilon_{k_1}-\epsilon_{k_2}+\hbar\omega_{el}}$

$$= -i \sum_{k_1 k_2 \sigma_1 \sigma_2 j} \left|B^j\right|^2 \frac{a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} \left[b_j, b^\dagger_{j'}\right]}{\epsilon_{k_1} - \epsilon_{k_2} + \hbar\omega_{el}}$$

$$i \sum_{k_1 k_2 \sigma_1 \sigma_2 j} \left|B^j\right|^2 \frac{\left[a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} b_j, a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_{j'}\right]}{\epsilon_{k_1} - \epsilon_{k_2} - \hbar\omega_{el}}$$

$$= -i \sum_{k_1 k_2 \sigma_1 \sigma_2 j} \left|B^j\right|^2 \frac{a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} \delta_{jj'}}{\epsilon_{k_1} - \epsilon_{k_2} + \hbar\omega_{el}}$$

and

$$i \sum_{k_1 k_2 \sigma_1 \sigma_2 j} \left|B^j\right|^2 \frac{\left[a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} b^\dagger_j, a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} b_{j'}\right]}{\epsilon_{k_1} - \epsilon_{k_2} - \hbar\omega_{el}}$$

$$= i \sum_{k_1 k_2 \sigma_1 \sigma_2 j} \left|B^j\right|^2 \frac{a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} \delta_{jj'}}{\epsilon_{k_1} - \epsilon_{k_2} - \hbar\omega_{el}}$$

$$\left[H', \tau\right] = i\left\{ \sum_{k_1 k_2 \sigma_1 \sigma_2 jj'} \left|B^j\right|^2 \frac{a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} \delta_{jj'}}{\epsilon_{k_1} - \epsilon_{k_2} - \hbar\omega_{el}} - \sum_{k_1 k_2 \sigma_1 \sigma_2 jj'} \left|B^j\right|^2 \frac{a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} a^\dagger_{mk_1\sigma_1} a_{nk_2\sigma_2} \delta_{jj'}}{\epsilon_{k_1} - \epsilon_{k_2} + \hbar\omega_{el}} \right\} \tag{4.2.7}$$

The final result of the (4.2.7) is obtained by taking to account the energy conservation $\epsilon_{k_1} + \epsilon_{k_2} = \epsilon_{k_1 - \hbar k} + \epsilon_{k_2 + \hbar k}$ [23] and if $j = j'$ we get

$$\left[H', \tau\right] = -2i \sum_{k_1 k_2 \sigma_1 \sigma_2} \frac{\hbar\omega_{el} \left|B^j\right|^2 a^\dagger_{mk_1\sigma_1} a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} a_{nk_2\sigma_2}}{\left(\epsilon_{k_1} - \epsilon_{k_2}\right)^2 - \left(\hbar\omega_{el}\right)^2} \tag{4.2.8}$$

Then, eq(4.2.2) becomes

$$H = \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_j \hbar\omega_{el} b^\dagger_j b_j + \sum_{k_1 k_2 \sigma_1 \sigma_2} \frac{\hbar\omega_{el} \left|B^j\right|^2 a^\dagger_{mk_1\sigma_1} a^\dagger_{nk_2\sigma_2} a_{mk_1\sigma_1} a_{nk_2\sigma_2}}{\left(\epsilon_{k_1} - \epsilon_{k_2}\right)^2 - \left(\hbar\omega_{el}\right)^2} \tag{4.2.9}$$

The Hamiltonian for the lower of two level system has well known BCS form for $\epsilon_{k_1} = \epsilon_{k_2}$ and for single layer band or orbital $m = n$ [1].

A two level system can be described by pseudo spin($s = 1/2$) formalism, because for every two level system all 2×2 matrices and spin-half pauli matrices along with 2×2 unit matrix form a complete set in the space of herimitian 2×2 matrices [4].

Then, eq(4.2.9) becomes

$$H = \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_j \hbar\omega_{el} b^\dagger_j b_j - \sum_{kk'} \frac{|B^j|^2}{\hbar\omega_{el}} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow} \tag{4.2.10}$$

4.2.1 For conduction electron

Consider the Hamiltonian H as [1,33]

$$H = \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_j \hbar\omega_{el} b^\dagger_j b_j - \sum_{kk'} \frac{|B^j|^2}{\hbar\omega_{el}} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow} \tag{4.2.11}$$

4.2.2 Equation of motion

Now we need to find equation of motion for Green's functions $G_t = \langle\langle a_{k\uparrow}, a^\dagger_{k'\uparrow}\rangle\rangle$.

Equation of motion in Fourier transform of Green's functions is given by

$$\omega\langle\langle a_{k\uparrow}, a^\dagger_{k'\uparrow}\rangle\rangle = \langle [a_{k\uparrow}, a^\dagger_{k'\uparrow}]\rangle + \langle\langle [a_{k\uparrow}, H], a^\dagger_{k'\uparrow}\rangle\rangle \tag{4.2.12}$$

The laws of quantum mechanics provide that the annihilation operator a_k , and its hermitian conjugate the creation operator $a^\dagger_k$, obey the boson commutation relation.

$[a_k, a^\dagger_k] = a_k a^\dagger_k - a^\dagger_k a_k = 1$

$[a_k, a^\dagger_{k'}] = [b_k, b^\dagger_{k'}] = [\alpha_k, \alpha^\dagger_{k'}] = [\beta_k, \beta^\dagger_{k'}] = \delta_{kk'} = 1$ if $k = k'$ otherwise 0 and $[a_k, a_k] = [a^\dagger_k, a^\dagger_k] = [a_{k\uparrow}, a_{k'\downarrow}] = o$

$$\omega\langle\langle a_{k\uparrow}, a^\dagger_{k'\uparrow}\rangle\rangle = 1 + \langle\langle [a_{k\uparrow}, H], a^\dagger_{k'\uparrow}\rangle\rangle \tag{4.2.13}$$

We need to evaluate $[a_{k\uparrow}, H]$

$[a_{k\uparrow}, H] = [a_{k\uparrow}, H_o] + [a_{k\uparrow}, H_{int}]$

$[a_{k\uparrow}, H_o] = [a_{k\uparrow}, \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_j \hbar\omega_{el} b^\dagger_j b_j]$

$= [a_{k\uparrow}, \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma}] + [a_{k\uparrow}, \sum_j \hbar\omega_{el} b^\dagger_j b_j]$

$= \sum_{pk\sigma} \epsilon_k [a_{p\uparrow}, a^\dagger_{k\sigma} a_{k\sigma}] + \sum_{kj} \hbar\omega_{el} [a_{k\uparrow}, b^\dagger_j b_j]$

$= \sum_{pk\sigma} \epsilon_k a_{k\sigma} [a_{p\uparrow}, a^\dagger_{k\sigma}] + 0$

$= \epsilon_k \delta_{pk} \delta_{\sigma\uparrow} a_{k\sigma}$

If $\sigma =\uparrow$ and $p = k$ we can get

$$[a_{k\uparrow}, H_o] = \epsilon_k a_{k\uparrow} \tag{4.2.14}$$

and for $\left[a_{k\uparrow}, H_{int}\right]$

$\left[a_{k\uparrow}, H_{int}\right] = \left[a_{k\uparrow}, -\sum_{kk'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}\right]$

$= -\sum_{pp'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} \left[a_{p\uparrow}, a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow}\right]$

$= -\sum_{pp'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} \left[a_{p\uparrow}, a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\downarrow}\right] a_{p'\downarrow} a_{-p'\uparrow} + a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\downarrow} \left[a_{p\uparrow}, a_{p'\downarrow} a_{-p'\uparrow}\right]$

$= -\sum_{pp'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} \delta_{pp'} \delta_{\uparrow\uparrow} a^{\dagger}_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow} = -\sum_{kk'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} \delta_{kk'} \delta_{\uparrow\uparrow} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}$

If $p = k$, $p' = k'$and $p = p'$ then, $k = k'$ therefore $\left[a_{k\uparrow}, H_{int}\right]$ becomes

$$\left[a_{k\uparrow}, H_{int}\right] = -\sum_{kk'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow} \tag{4.2.15}$$

Substituting eq(4.2.14) and eq(4.2.15) into eq(4.2.13) we get

$$\omega\left\langle\left\langle a_{k\uparrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle = 1 + \left\langle\left\langle \epsilon_k a_{k\uparrow} - \sum_{kk'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle \tag{4.2.16}$$

$\left\langle\left\langle \epsilon_k a_{k\uparrow} - \sum_{kk'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle = \left\langle\left\langle \epsilon_k a_{k\uparrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle - \left\langle\left\langle \sum_{kk'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle$

Using Wick's decoupling theorem

$\left\langle\left\langle a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle = \left\langle a_{k'\downarrow} a_{-k'\uparrow}\right\rangle \left\langle\left\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle$, then equation of motiom for the first case becomes

$$\left(\omega - \epsilon_k\right)\left\langle\left\langle a_{k\uparrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle = 1 - \sum_{kk'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} \left\langle a_{k'\downarrow} a_{-k'\uparrow}\right\rangle \left\langle\left\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle \tag{4.2.17}$$

let

$\Delta = \sum_{k'} \frac{\left|B^j\right|^2}{\hbar\omega_{el}} \left\langle a_{k'\downarrow} a_{-k'\uparrow}\right\rangle$

$$\left(\omega - \epsilon_k\right)\left\langle\left\langle a_{k\uparrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle = 1 - \Delta\left\langle\left\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle \tag{4.2.18}$$

We can use a similar way to find equation of motion for Green's functions $G_t = \left\langle\left\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle$ eq(4.2.12) can be written as

$$\omega\left\langle\left\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle = \left\langle\left[a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\right]\right\rangle + \left\langle\left\langle\left[a^{\dagger}_{-k\downarrow}, H\right], a^{\dagger}_{k'\uparrow}\right\rangle\right\rangle \tag{4.2.19}$$

To solve eq(4.2.19) let us calculate $\big[a^\dagger_{-k\downarrow}, H\big]$

$\big[a^\dagger_{-k\downarrow}, H\big] = \big[a^\dagger_{-k\downarrow}, H_o\big] + \big[a^\dagger_{-k\downarrow}, H_{int}\big]$

The first term can be evaluated

$\big[a^\dagger_{-k\downarrow}, H_o\big] = \big[a^\dagger_{-k\downarrow}, \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{K\sigma}\big] + \big[a^\dagger_{-k\downarrow}, \sum_j \hbar\omega_{el} b^\dagger_j b_j\big]$

$= \sum_{pk\sigma} \epsilon_p \big[a^\dagger_{-k\downarrow}, a^\dagger_{p\sigma} a_{p\sigma}\big] + \sum_{jk} \hbar\omega_{el} \big[a^\dagger_{-k\downarrow}, b^\dagger_j b_j\big]$

$= \sum_{pk\sigma} \epsilon_p \big[a^\dagger_{-k\downarrow}, a_{p\sigma}\big] a^\dagger_{p\sigma} + 0$

If $p = -k$, $\sigma =\downarrow$ and since $\epsilon_{-k} = \epsilon_k$ is the kinetic energy of conduction electrons.

$$\big[a^\dagger_{-k\downarrow}, H_o\big] = -\epsilon_k a^\dagger_{-k\downarrow} \tag{4.2.20}$$

and the second term also evaluated

$\big[a^\dagger_{-k\downarrow}, H_{int}\big] = \big[a^\dagger_{-k\downarrow}, -\sum_{kk'} \frac{|B^j|^2}{\hbar\omega_{el}} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}\big]$

$= -\sum_{kk'p} \frac{|B^j|^2}{\hbar\omega_{el}} \big[a^\dagger_{-k\downarrow}, a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{k'\downarrow} a_{-k'\uparrow}\big]$

$= -\sum_{kk'p} \frac{|B^j|^2}{\hbar\omega_{el}} \Big[a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} \big\{a^\dagger_{-k\downarrow}, a_{k'\downarrow}\big\} a_{-k'\uparrow} - a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{k'\downarrow} \big\{a^\dagger_{-k\downarrow}, a_{-k'\uparrow}\big\}\Big]$

$= -\sum_{kk'p} \frac{|B^j|^2}{\hbar\omega_{el}} a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} \delta_{-kk'} \delta_{\downarrow\downarrow} a_{-k'\uparrow}$

If $k' = -k$ and $p = k$ we get

$$\big[a^\dagger_{-k\downarrow}, H_{int}\big] = -\sum_{kk'} \frac{|B^j|^2}{\hbar\omega_{el}} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{k\uparrow} \tag{4.2.21}$$

Substituting eq(4.2.20) and eq(4.2.21) into eq(4.2.19) gives

$$\omega\big\langle\big\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\big\rangle\big\rangle = \big\langle\big\langle -\epsilon_k a^\dagger_{-k\downarrow} - \sum_{kk'} \frac{|B^j|^2}{\hbar\omega_{el}} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{k\uparrow}, a^\dagger_{k'\uparrow}\big\rangle\big\rangle \tag{4.2.22}$$

Then, equation of motion for second case is

$$\big(\omega + \epsilon_k\big)\big\langle\big\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\big\rangle\big\rangle = -\sum_{kk'} \frac{|B^j|^2}{\hbar\omega_{el}} \big\langle a^\dagger_{-k\downarrow} a^\dagger_{k\uparrow}\big\rangle\big\langle\big\langle a_{k\uparrow}, a^\dagger_{k'\uparrow}\big\rangle\big\rangle \tag{4.2.23}$$

$\Delta = \sum_k \frac{|B^j|^2}{\hbar\omega_{el}} \big\langle a^\dagger_{-k\downarrow} a^\dagger_{k\uparrow}\big\rangle$

$$\big(\omega + \epsilon_k\big)\big\langle\big\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\big\rangle\big\rangle = -\Delta\big\langle\big\langle a_{k\uparrow}, a^\dagger_{k'\uparrow}\big\rangle\big\rangle \tag{4.2.24}$$

The final results of equation of motion for these two case are summarized by

$$\Big(\omega - \epsilon_k\Big)\Big\langle\Big\langle a_{k\uparrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle = 1 - \Delta\Big\langle\Big\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle \tag{4.2.25}$$

$$\Big(\omega + \epsilon_k\Big)\Big\langle\Big\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle = -\Delta\Big\langle\Big\langle a_{k\uparrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle \tag{4.2.26}$$

$\Big\langle\Big\langle a_{k\uparrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle = \frac{1-\Delta\Big\langle\Big\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle}{\omega-\epsilon_k}$

Substituting this in eq(4.2.25) we get

$\Big\langle\Big\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle = -\frac{\Delta}{\omega^2-\epsilon_k^2}\Bigg[1 - \Delta\Big\langle\Big\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle\Bigg]$

$\Big(1 - \frac{\Delta^2}{\omega^2-\epsilon_k^2}\Big)\Big\langle\Big\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle = -\frac{\Delta}{\omega^2-\epsilon_k^2}$

$$\Big\langle\Big\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle = -\frac{\Delta}{\omega^2 - \epsilon_k^2 - \Delta^2} \tag{4.2.27}$$

The superconductivity energy gap Δ parameter is defined as

$$\Delta = \frac{V}{\beta}\sum_{kk'}\Big\langle\Big\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\Big\rangle\Big\rangle \tag{4.2.28}$$

Where $V = \frac{\Big|B^j\Big|^2}{\hbar\omega_{el}}$

Substituting eq(4.2.27) into eq (4.2.28)

$$\Delta = \frac{V}{\beta}\sum_{kk'} -\frac{\Delta}{\omega^2 - \epsilon_k^2 - \Delta^2} \tag{4.2.29}$$

$\omega \longrightarrow i\omega_n$ and using the Matsubara frequency

$\omega_n = \frac{\Big(2n+1\Big)\pi}{\beta}$

$$1 = \frac{V}{\beta}\sum_{kk'}\frac{\beta^2}{\Bigg(\Big(2n+1\Big)\pi\Bigg)^2 + \epsilon_k^2\beta^2 + \Delta^2\beta^2} \tag{4.2.30}$$

$$1 = V\beta\sum_{kk'}\frac{1}{\Bigg(\Big(2n+1\Big)\pi\Bigg)^2 + \Bigg(\epsilon_k^2 + \Delta^2\Bigg)\beta^2} \tag{4.2.31}$$

Assuming that $E^2 = \epsilon_k^2 + \Delta^2$

$$1 = V\beta\sum_{kk'}\frac{1}{\Bigg(\Big(2n+1\Big)\pi\Bigg)^2 + E^2\beta^2} \tag{4.2.32}$$

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

Where $x = E\beta$

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

Then, eq(4.2.32) becomes

$$1 = V\beta\sum_k \frac{1}{2E\beta}tanh(\frac{E\beta}{2}) \tag{4.2.33}$$

$$1 = 2N(o)V\beta\int_0^{\hbar\omega_{el}} \frac{1}{2\beta E}tanh(\frac{E\beta}{2})dE \tag{4.2.34}$$

$$1 = N(o)V\int_0^{\hbar\omega_{el}} \frac{tanh\left(\frac{E\beta}{2}\right)}{E}dE \tag{4.2.35}$$

$\beta = \frac{1}{K_BT}$

$$1 = N(o)V\int_0^{\hbar\omega_{el}} \frac{tanh\left(\frac{E}{2K_BT}\right)}{E}dE \tag{4.2.36}$$

Let $x = \frac{E}{2K_BT}$,$E = 2K_BTx$ and $dE = 2K_BTdx$

Then, eq(4.2.35) becomes for superconductors $T = T_c$

$$1 = N(o)V\int_0^{\frac{\hbar\omega_{el}}{2K_BT_c}} \frac{tanhx}{x}dx \tag{4.2.37}$$

Let $u = tanhx$,$dv = \frac{1}{x}dx$ $du = sec^2xdx$ and $v = lnx$

$\int_0^{\frac{\hbar\omega_{el}}{2K_BT_c}} \frac{tanhx}{x}dx = lnxtanhx\Big|_0^{\hbar\omega_{el}/2K_BT_c} - \int_0^{\frac{\hbar\omega_{el}}{2K_BT_c}} sec^2xlnxdx$

$$1 = N(o)V\left[lnxtanhx\Big|_0^{\hbar\omega_{el}/2K_BT_c} - \int_0^{\frac{\hbar\omega_{el}}{2K_BT_c}} sec^2xlnxdx\right] \tag{4.2.38}$$

$$\frac{1}{N(o)V} = lnxtanhx\Big|_0^{\hbar\omega_{el}/2K_BT_c} - \int_0^{\frac{\hbar\omega_{el}}{2K_BT_c}} sec^2xlnxdx \tag{4.2.39}$$

Extend the upper limit of the integral to infinity that mean

$\int_0^{\infty} sec^2xlnxdx \approx ln(0.44)$ and $tanhx \approx 1$

$$\frac{1}{N(o)V} = ln\big(\frac{\hbar\omega_{el}}{2K_BT_c}\big) - ln\big(0.44\big) \qquad (4.2.40)$$

$$N(o)V = N(o)\frac{\left|B^j\right|^2}{\hbar\omega_{el}} = \lambda_{el}$$

$$K_BT_c = 1.14\hbar\omega_{el}e^{-\frac{1}{\lambda_{el}}} \qquad (4.2.41)$$

This is well known BCS form of superconductivity theory.

4.3 Phonon-exciton combined Mechanism

A combined phonon-exciton mechanism explain the T_c values very well as it is believed that for superconductors the coupling strong as result phonon alone can not explain high critical temperature discussed by many people [1-4].

The Hamiltonian of a system of conduction electron interacting with phonons (Phonon-exciton) described by the two level system can be written [4, 33]

$$H = H_e + H_{ph} + H_{e-ph} + H_c \qquad (4.3.1)$$

Where

$H_e = \sum_{k\sigma} \epsilon_k a^{\dagger}_{k\sigma} a_{k\sigma}$

ϵ_k is the single energy of electron in the conduction band. $a^{\dagger}_{k\sigma}$ and $a_{k\sigma}$ are the usual creation and annihilation operators. k being the wave vector and σ is spin index.

H_{ph} is the standard phonon Hamiltonian, which can be written as

$H_{ph} = -\sum_{kk'} V_{ph} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}$

H_{e-ph} is the electron-phonon interaction Hamiltonian,which can be written as

$H_{e-ph} = -\sum_{kk'} V_{el} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}$ and

H_c is the screened coulomb interaction between conduction electrons

$H_c = \sum_{kk'} V_c a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}$

The final form of pairing interaction is obtained by [3]

$$H = \sum_{k\sigma} \epsilon_k a_{k\sigma}^{\dagger} a_{k\sigma} - \sum_{kk'} \big(V_{ph} + V_{el} - V_c\big) a_{k\uparrow}^{\dagger} a_{-k\downarrow}^{\dagger} a_{k'\downarrow} a_{-k'\uparrow} \tag{4.3.2}$$

Where

V_{ph} is the phonon-induced interaction.V_{el} is the electron-induced interaction. And V_c is the screened coulomb repulsion between conduction electron.

Now we need to find equation of motion for Green's function

$G_t = \big\langle\big\langle a_{k\uparrow}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle$

$$\omega\big\langle\big\langle a_{k\uparrow}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle = 1 + \big\langle\big\langle \big[a_{k\uparrow}, H\big], a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle \tag{4.3.3}$$

$\big[a_{k\uparrow}, H\big] = \big[a_{k\uparrow}, \sum_{p\sigma} \epsilon_p a_{p\sigma}^{\dagger} a_{p\sigma}\big] + \big[a_{k\uparrow}, -\sum_{pk'} \big(V_{ph} + V_{el} - V_c\big) a_{p\uparrow}^{\dagger} a_{-p\downarrow}^{\dagger} a_{k'\downarrow} a_{-k'\uparrow}\big]$

at$p = k$

Using eq(4.2.14) and eq(4.2.15)

$$\big[a_{k\uparrow}, H\big] = \epsilon_k a_{k\uparrow} - \sum_{kk'} \big(V_{ph} + V_{el} - V_c\big) a_{-k\downarrow}^{\dagger} a_{k'\downarrow} a_{-k'\uparrow} \tag{4.3.4}$$

Equation of motion becomes

$$\omega\big\langle\big\langle a_{k\uparrow}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle = 1 + \big\langle\big\langle \epsilon_k a_{k\uparrow} - \sum_{kk'} \big(V_{ph} + V_{el} - V_c\big) a_{-k\downarrow}^{\dagger} a_{k'\downarrow} a_{-k'\uparrow}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle \tag{4.3.5}$$

Using Wick's decoupling theorem

$\big\langle\big\langle a_{-k\downarrow}^{\dagger} a_{k'\downarrow} a_{-k'\uparrow}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle = \big\langle a_{k'\downarrow} a_{-k'\uparrow}\big\rangle\big\langle\big\langle a_{-k\downarrow}^{\dagger}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle$

$$\big(\omega - \epsilon_k\big)\big\langle\big\langle a_{k\uparrow}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle = 1 - \sum_{kk'} \big(V_{ph} + V_{el} - V_c\big)\big\langle a_{k'\downarrow} a_{-k'\uparrow}\big\rangle\big\langle\big\langle a_{-k\downarrow}^{\dagger}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle \tag{4.3.6}$$

The gap function is

$\Delta = \sum_{kk'} \big(V_{ph} + V_{el} - V_c\big)\big\langle a_{k'\downarrow} a_{-k'\uparrow}\big\rangle$

Therefore equation of motion is

$$\big(\omega - \epsilon_k\big)\big\langle\big\langle a_{k\uparrow}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle = 1 - \Delta\big\langle\big\langle a_{-k\downarrow}^{\dagger}, a_{k'\uparrow}^{\dagger}\big\rangle\big\rangle \tag{4.3.7}$$

In similar way we need to find equation of motion for Green's function $G_t = \langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle$

$$\omega\langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle = \langle [a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}]\rangle + \langle\langle [a^\dagger_{-k\downarrow}, H], a^\dagger_{k'\uparrow}\rangle\rangle \tag{4.3.8}$$

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

$$\omega\langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle = \langle\langle [a^\dagger_{-k\downarrow}, H], a^\dagger_{k'\uparrow}\rangle\rangle \tag{4.3.9}$$

$[a^\dagger_{-k\downarrow}, H] = [a^\dagger_{-k\downarrow}, \sum_{k\sigma} a^\dagger_{k\sigma} a_{k\sigma}] + [a^\dagger_{-k\downarrow}, -\sum_{kk'} (V_{ph} + V_{el} - V_c) a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}]$

Using eq(4.2.20) and eq(4.2.21) $[a^\dagger_{-k\downarrow}, H]$

$$[a^\dagger_{-k\downarrow}, H] = -\epsilon_k a^\dagger_{-k\downarrow} - \sum_{kk'} (V_{ph} + V_{el} - V_c) a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{k\uparrow} \tag{4.3.10}$$

Using Wick's decoupling theorem

$\langle\langle a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{k\uparrow}, a^\dagger_{k'\uparrow}\rangle\rangle = \langle a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}\rangle \langle\langle a_{k\uparrow}, a^\dagger_{k'\uparrow}\rangle\rangle$

$$(\omega + \epsilon_k)\langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle = -\sum_{kk'} (V_{ph} + V_{el} - V_c)\langle a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}\rangle \langle\langle a_{k\uparrow}, a^\dagger_{k'\uparrow}\rangle\rangle \tag{4.3.11}$$

The gap function is

$\Delta = \sum_{kk'} (V_{ph} + V_{el} - V_c)\langle a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}\rangle$

$$(\omega + \epsilon_k)\langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle = -\Delta\langle\langle a_{k\uparrow}, a^\dagger_{k'\uparrow}\rangle\rangle \tag{4.3.12}$$

From eq(4.3.7) we get

$$\langle\langle a_{k\uparrow}, a^\dagger_{k'\uparrow}\rangle\rangle = \frac{1 - \Delta\langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle}{\omega - \epsilon_k} \tag{4.3.13}$$

substituting eq(4.3.13) into eq(4.3.12) we get

$$\langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle = -\Delta\left(\frac{1 - \Delta\langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle}{\omega^2 - \epsilon_k^2}\right) \tag{4.3.14}$$

From eq(4.3.14)

$$\langle\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\rangle\rangle = -\frac{\Delta}{\omega^2 - \epsilon_k^2 - \Delta^2} \tag{4.3.15}$$

The superconductivity energy gap parameter is defined as

$\Delta = \frac{U}{\beta}\sum_{kk'}\langle\langle a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k'\uparrow}\rangle\rangle$

Where

$U = V_{ph} + V_{el} - V_c$

$$\Delta = \frac{U}{\beta}\sum_{kk'} -\frac{\Delta}{\omega^2 - \epsilon_k^2 - \Delta^2} \tag{4.3.16}$$

$\omega \longrightarrow i\omega_n$ and using Matsubara frequency $\omega_n = \frac{\left(2n+1\right)\pi}{\beta}$

$\omega \longrightarrow i\frac{\left(2n+1\right)\pi}{\beta}$

$$\Delta = \frac{U}{\beta}\sum_{kk'} -\frac{\Delta}{\left[i\frac{\left(2n+1\right)\pi}{\beta}\right]^2 - \epsilon_k^2 - \Delta^2} \tag{4.3.17}$$

$$\Delta = \frac{U}{\beta}\sum_{kk'} \frac{\Delta\beta^2}{\left[\left(2n+1\right)\pi\right]^2 + \epsilon_k^2\beta^2 + \Delta^2\beta^2} \tag{4.3.18}$$

$E = \sqrt{\epsilon_k^2 + \Delta^2}$

$$1 = U\beta\sum_{kk'} \frac{1}{\left[\left(2n+1\right)\pi\right]^2 + E^2\beta^2} \tag{4.3.19}$$

Using relation

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

Where

$x = E\beta$

$$1 = U\beta\sum_{k} \frac{1}{2E\beta}tanh\left(\frac{E\beta}{2}\right) \tag{4.3.20}$$

$$1 = 2N(o)U\int_0^{\hbar\omega_{e-ph}} \frac{1}{2E}tanh\left(\frac{E\beta}{2}\right)dE \tag{4.3.21}$$

$$1 = N(o)U\int_0^{\hbar\omega_{e-ph}} \frac{tanh\left(\frac{E\beta}{2}\right)}{E}dE \tag{4.3.22}$$

$\beta = \frac{1}{K_B T_c}$ where K_B is Boltzmann constant and T_c is critical(transition) temperature

$$1 = N(o)U\int_0^{\hbar\omega_{e-ph}} \frac{tanh\left(\frac{E}{2K_B T_c}\right)}{E}dE \tag{4.3.23}$$

$$\frac{1}{N(o)U} = \int_0^{\hbar\omega_{e-ph}} \frac{tanh\left(\frac{E}{2K_BT_c}\right)}{E} dE \qquad (4.3.24)$$

Where $U = V_{ph} + V_{el} - V_c$

$$\frac{1}{N(o)\left(V_{ph} + V_{el} - V_c\right)} = \int_0^{\hbar\omega_{e-ph}} \frac{tanh\left(\frac{E}{2K_BT_c}\right)}{E} dE \qquad (4.3.25)$$

let

$x = \frac{E}{2K_BT_c}$,$E = 2K_BT_cx$ and $dE = 2K_BT_cdx$

$$\frac{1}{N(o)\left(V_{ph} + V_{el} - V_c\right)} = \int_0^{\hbar\omega_{e-ph}/2K_BT_c} \frac{tanh\left(x\right)}{2K_BT_cx} 2K_BT_cdx \qquad (4.3.26)$$

$$\frac{1}{N(o)\left(V_{ph} + V_{el} - V_c\right)} = \int_0^{\hbar\omega_{e-ph}/2K_BT_c} \frac{tanh\left(x\right)}{x} dx \qquad (4.3.27)$$

let

$u = tanh\left(x\right)$, $du = sech^2(x)$

$dv = \frac{1}{x}dx$ and $v = lnx$

$$\frac{1}{N(o)\left(V_{ph} + V_{el} - V_c\right)} = ln(x)tanh(x)\Big|_0^{\hbar\omega_{e-ph}/2K_BT_c} - \int_0^{\hbar\omega_{e-ph}/2K_BT_c} sech^2xlnxdx \qquad (4.3.28)$$

Extend the upper limit of the integral to infinity that mean

$\int_0^{\infty} sech^2xlnxdx \approx ln(0.44)$ and $tanhx \approx 1$

$$\frac{1}{N(o)\left(V_{ph} + V_{el} - V_c\right)} = lnx - ln(0.44) \qquad (4.3.29)$$

$$e^{\frac{1}{N(o)\left(V_{ph}+V_{el}-V_c\right)}} = 1.14\frac{\hbar\omega_{e-ph}}{K_BT_c} \qquad (4.3.30)$$

$$T_c = 1.14\frac{\hbar\omega_{e-ph}}{K_B} e^{\left(-\frac{1}{N(o)\left(V_{ph}+V_{el}-V_c\right)}\right)} \qquad (4.3.31)$$

Assuming that $\frac{\hbar}{K_B} = 1$ and $\omega_{e-ph} = \omega_{ph}^{r_{ph}}\omega_{el}^{r_{el}}$

$$T_c = 1.14\omega_{ph}^{r_{ph}}\omega_{el}^{r_{el}} e^{\left(-\frac{1}{N(o)\left(V_{ph}+V_{el}-V_c\right)}\right)} \qquad (4.3.32)$$

$N(o)V_{ph} = \lambda_{ph}$ is the phonon exciton coupling constant.

$N(o)V_{el} = \lambda_{el}$ is the electron(hole) exciton coupling constant. And

$N(o)V_c = \mu^*$ is the parameter arising from coulomb repulsion.

$$T_c = 1.14\omega_{ph}^{r_{ph}}\omega_{el}^{r_{el}}e^{-\frac{1}{\lambda_{ph}+\lambda_{el}-\mu^*}} \tag{4.3.33}$$

Where

$\lambda_{el}^* = \lambda_{el} - \mu^*$

$$T_c = 1.14\omega_{ph}^{r_{ph}}\omega_{el}^{r_{el}}e^{-\frac{1}{\lambda_{ph}+\lambda_{el}^*}} \tag{4.3.34}$$

If $\mu^* = 0$ that mean assuming that there is no screened repulsion.

$$T_c = 1.14\omega_{ph}^{r_{ph}}\omega_{el}^{r_{el}}e^{-\frac{1}{\lambda_{ph}+\lambda_{el}}} \tag{4.3.35}$$

If the parameter arising from coulomb repulsion(μ^*) has effect on both phonon and electron then transition temperature T_c to be

$$T_c = 1.14\omega_{ph}^{r_{ph}}\omega_{el}^{r_{el}}e^{-\frac{1}{\lambda_{ph}^*+\lambda_{el}^*}} \tag{4.3.36}$$

Where

$r_{ph} = \frac{\lambda_{ph}}{\lambda_{el}+\lambda_{ph}}$ and $r_{el} = \frac{\lambda_{el}}{\lambda_{ph}+\lambda_{el}}$

$\lambda_{ph}^* = \frac{\lambda_{ph}}{1+\lambda_{ph}}$ and $\lambda_{el}^* = \frac{\lambda_{el}}{1+\lambda_{el}}$

$\lambda_{ph}^* = \lambda_{ph} - \mu_{ph}^*$ and $\lambda_{el}^* = \lambda_{el} - \mu_{el^*}$

$\mu_{ph}^* = \frac{\lambda_{ph}^2}{1+\lambda_{ph}}$ and $\mu_{el}^* = \frac{\lambda_{el}^2}{1+\lambda_{el}}$

ω_{ph} and ω_{el} are energies of phononic and electronic excitation or cut off frequencies, in temperature units.

$N(o)$ is density of states at Fermi energy.

4.4 Superconductivity Energy Gap

Solution of the gap-equation at $T = 0$ can be evaluated as follows using eq(4.3.24) which becomes

$$\frac{1}{N(o)U} = \int_0^{\hbar\omega_{e-ph}} \frac{d\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2(0)}} \tag{4.4.1}$$

where we have assumed that $\hbar\omega_{e-ph} \ll E_F$ and

Using the relation of the following

$\int \frac{dx}{\sqrt{x^2+1}} = ln\big(x + \sqrt{x^2+1}\big)$

and using hyperbolic function

$\sinh^{-1}(x) = \tanh^{-1}\big(\frac{x}{\sqrt{x^2+1}}\big) = ln\big(x + \sqrt{x^2+1}\big)$

Where $x = \frac{\epsilon_k}{\Delta(0)}$

$\int_0^{\hbar\omega_{e-ph}} \frac{d\epsilon_k}{\sqrt{\epsilon_k^2+\Delta^2(0)}} = ln\left[\frac{\hbar\omega_{e-ph}+\sqrt{\hbar\omega_{e-ph}^2+\Delta^2(0)}}{\Delta(0)}\right] = Sinh^{-1}\big(\frac{\hbar\omega_{e-ph}}{\Delta(0)}\big)$

$ln\left[\frac{\hbar\omega_{e-ph}+\sqrt{\hbar\omega_{e-ph}^2+\Delta^2(0)}}{\Delta(0)}\right] \approx ln\left(\frac{2\hbar\omega_{e-ph}}{\Delta(0)}\right)$

Then eq(4.4.1) becomes

$$\frac{1}{N(o)U} \approx ln\left(\frac{2\hbar\omega_{e-ph}}{\Delta(0)}\right) \tag{4.4.2}$$

$$e^{\left(\frac{1}{N(o)U}\right)} \approx \frac{2\hbar\omega_{e-ph}}{\Delta(0)} \tag{4.4.3}$$

From above equation we can get

$$\Delta(0) \approx 2\hbar\omega_{e-ph} e^{\left(-\frac{1}{N(o)U}\right)} \tag{4.4.4}$$

4.5 Temperature dependent energy gap

To obtain temperature dependent energy gap of eq(4.3.24), we used the technique to solve the integral

$$\frac{1}{N(o)U} = \int_0^{\hbar\omega_{e-ph}} dE \frac{1}{\sqrt{\epsilon_k^2 + \Delta^2}} \tanh\left(\beta\frac{\sqrt{\epsilon_k^2 + \Delta^2}}{2}\right) \tag{4.5.1}$$

$N(o)U = \lambda$

$$\frac{1}{\lambda} = \ln(1.14\frac{\hbar\omega_{e-ph}}{k_B T}) - \Delta^2 \frac{1}{(\pi k_B T)^2}\frac{8.414}{8} + - - - -- \tag{4.5.2}$$

but for BCS $T = T_c$

$\frac{1}{\lambda} = \ln(1.14\frac{\hbar\omega_{e-ph}}{k_B T_c})$ and assuming the above equations yields that

$$\ln(\frac{T}{T_c}) = -\Delta^2 \frac{1}{(\pi k_B T_c)^2}\frac{8.414}{8} + - - - -- \tag{4.5.3}$$

using $\ln(1-x) = -x - \frac{x^2}{2} + - - - - - - - - --$

implies

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

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

implies

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

Hence

$$\Delta(T) = 3.06 k_B T_c \left(1 - \frac{T}{T_c}\right)^{1/2} \tag{4.5.4}$$

From BCS theory $\Delta(0) \approx 2K_B T_c$

Then

$$\Delta(T) = 1.53\Delta(0)\left(1 - \frac{T}{T_c}\right)^{1/2} \tag{4.5.5}$$

$$\frac{\Delta(T)}{\Delta(0)} = 1.53\left(1 - \frac{T}{T_c}\right)^{1/2} \tag{4.5.6}$$

The following table show that the transition temperature T_c of the experimental and theoretical values for $\lambda_{ph} = 0.3$, $\omega_{ph} = 300K$, $\omega_{el} = 4000K$ and for different values of λ_{el} using eq(4.3.35)

compunds	λ_{el}	experimental T_c(K)	theoretical T_c(K)	$\Delta(0)$ in mev	$\frac{2\Delta(0)}{K_B T_c}$
$LaO_{1-x}F_xFeAs$	0.048	26	27.5	6.57	3.99
$Ba_{1-x}K_xFe_2As_2$	0.074	38	39.4	9.42	4.00
$Fe_{1-y}Se_xTe_{1-x}$	0.015	15	16.2	3.87	3.99

Table 4.1: The calculated values of T_c, energy gap $\Delta(0)$ and reduced energy gap $\frac{2\Delta(0)}{K_B T_c}$ for different λ_{el} using eq(4.3.35)

The following table show that the transition temperature T_c of the experimental and theoretical values for $\lambda_{ph} = 0.3$, $\omega_{ph} = 300K$, $\omega_{el} = 4000K$ and for different values of λ_{el} using eq(4.3.36)

compunds	λ_{el}	experimental T_c(K)	theoretical T_c(K)	$\Delta(0)$ in mev	$\frac{2\Delta(0)}{K_B T_c}$
$LaO_{1-x}F_xFeAs$	0.0947	26	27.15	6.49	4.00
$Ba_{1-x}K_xFe_2As_2$	0.126	38	39.5	9.44	4.00
$Fe_{1-y}Se_xTe_{1-x}$	0.06	15	16.15	3.86	3.99

Table 4.2: The calculated values of T_c, energy gap $\Delta(0)$ and reduced energy gap $\frac{2\Delta(0)}{K_B T_c}$ for different λ_{el} using eq(4.3.36)

Chapter 5

Results and Discussion

5.1 Results

In chapter three (in the methodology part) we have used a quantum field theory by using Green's function techniques to develop the Green's function formalism by using equation of motion.

In the next chapter (or chapter four) in the first section (4.1) we have studied the effect of the electronic excitation (exciton mechanism) on electron pair formulation. In this mechanism the phonon coupling constant assuming zero ($\lambda_{ph} = 0$) and $\lambda_{el} \neq 0$. For this purpose we have studied a Hamiltonian which involving exciton-mechanism. We have reduced the Hamiltonian of the system canonically to obtain BCS type attractive pair interaction. Using this reduced Hamiltonian and applying Green's functions formalism we get an expression for T_c eq(4.2.41). This equation show that well known BCS theory of superconductivity.

The other of our study in section (4.3) we have investigated the effect of electron-phonon and electron-exciton coupling (phonon-exciton combined mechanism) to obtain transition temperature T_c. Similarly we have used Green's functions formalism . In this mechanism phonon coupling constant ($\lambda_{ph} \neq 0$) and electron coupling constant ($\lambda_{el} \neq 0$), as a result we get an expression for transition temperature T_c which have described in eq(4.3.35) and (4.3.36). Using these expressions we have calculated the transition temperature for selected sample of Iron-based superconductors (ferropnictides). For these two cases ω_{ph}, ω_{el} and λ_{ph} have the same values, λ_{el} is different with appropriate values.We have calculated the theoretical values of transition temperature T_c and reduced gap $\frac{2\Delta(0)}{K_B T_c}$ shown in table(4.1) and (4.2). The result show a slight differences when we compare with experimental values, but they are appropriate with each other.

The following graphs have been sketched using eq(4.3.35) and the data which listed in table(4.1)

Graph for $LaO_{1-x}F_xFeAs$

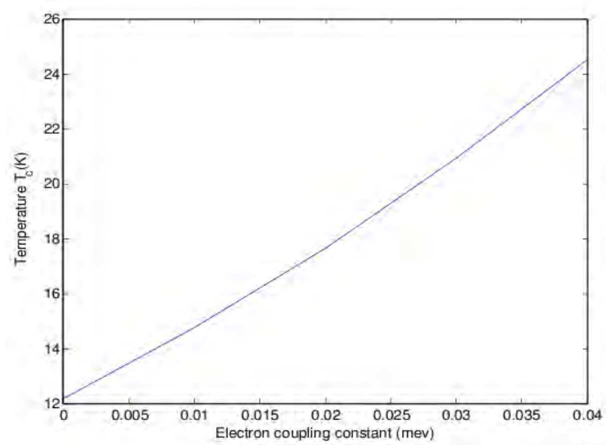

Figure 5.1: Electron coupling constant λ_{el} (mev) Vs Superconducting temperature T_c(K) for $LaO_{1-x}F_xFeAs$ superconductor.

Graph for $Ba_{1-x}K_xFe_2As_2$

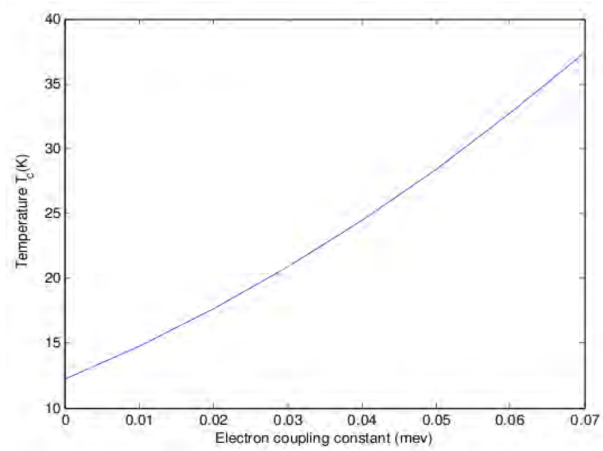

Figure 5.2: Electron coupling constant λ_{el} (mev) Vs Superconducting temperature T_c(K) for $Ba_{1-x}K_xFe_2As_2$ superconductor.

Graph for $Fe_{1-y}Se_xTe_{1-x}$

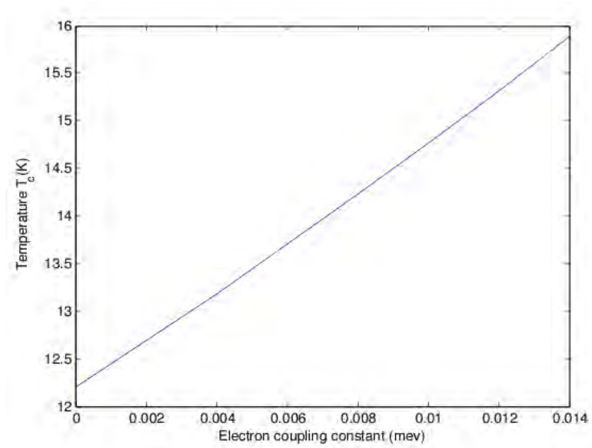

Figure 5.3: Electron coupling constant λ_{el} (mev) Vs Superconducting temperature T_c(K) for $Fe_{1-y}Se_xTe_{1-x}$ superconductor.

As seen in above graphs, when the electron coupling constant λ_{el} increases the superconducting temperature T_c also increases and enhance its maximum value.

The following graphs have been sketched using eq(4.5.5)

Graph for $LaO_{1-x}F_xFeAs$

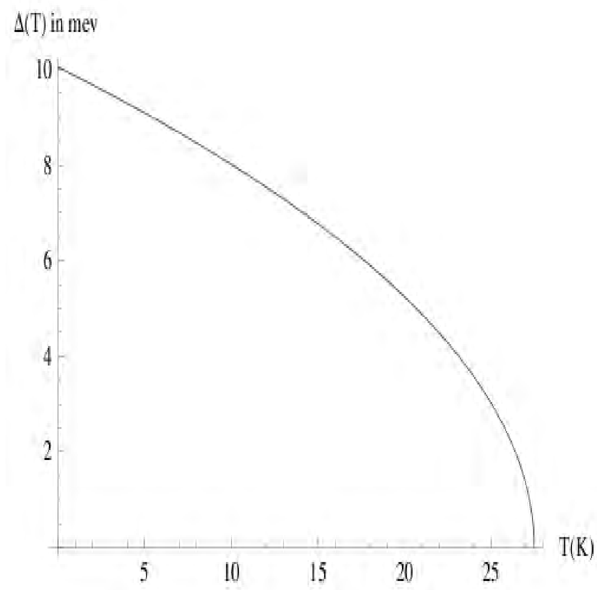

Figure 5.4: Temperature T(K) Vs Superconducting order parameter $\Delta(T)$(mev) for $LaO_{1-x}F_xFeAs$ superconductor.

Graph for $Ba_{1-x}K_xFe_2As_2$

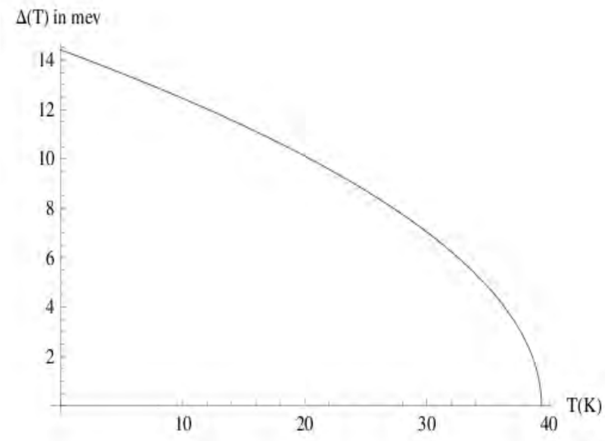

Figure 5.5: Temperature T(K) Vs Superconducting order parameter $\Delta(T)$(mev) for $Ba_{1-x}K_xFe_2As_2$ superconductor.

Graph for $Fe_{1-y}Se_xTe_{1-x}$

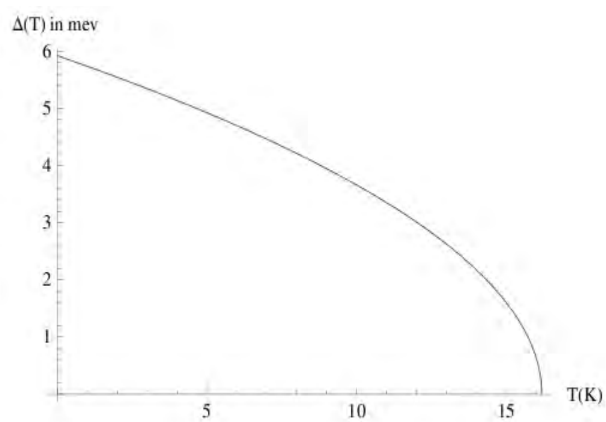

Figure 5.6: Temperature T(K) Vs Superconducting order parameter $\Delta(T)$(mev) for $Fe_{1-y}Se_xTe_{1-x}$ superconductor.

As seen in above figures , when the temperature increases the superconducting order parameter decreases and vanish as the temperature is equal to the critical temperature.

5.2 Discussion

The superconductivity in these newly discovered Iron-based superconductors (Iron pnictides compounds) is very important as these compounds contain magnetic element Iron(Fe). The parent compound which was discovered in 2008 by Kamihara et al, shows antiferromagnetic order below certain temperature T. In this recently discovered pnictide compounds superconductivity is induced by substitution of suitable amount of F on O site. The parent compound is unstable in its ground state. The instability caused due to presence of degenerate Fe 3d orbital.

The calculated values of gap parameter and superconducting transition temperature T_c almost coincide with experimental values. The values of reduced gap $\frac{2\Delta(0)}{K_B T_c}$ are substantially larger than the BCS value, which reveals the strong coupling effects are important and the mechanism of superconducting is different from BCS. While electron coupling constant λ_{el} increase the T_c is enhanced. The enhancement of T_c can be made by either electrons or holes doping.

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Declaration

This thesis is my original work, has not been presented for a degree in any other University and that all the sources of material used for the thesis have been dully acknowledged.

Name: Tesfaye Chebelew

Signature:− − − − − − − − − − − −

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This thesis has been submitted for examination with my approval as University advisor.

Name: Prof. P. Singh

Signature:− − − − − − − − − −−