SUPERCONDUCTIVITY AND JAHN TELLER EFFECT IN $LA(O_{1-X}F_X)FEAS$ SUPERCONDUCTOR

By

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Abstract

The recent discovery of superconductivity at moderately high temperature(26K to 55K) in doped iron-based pnictides($RnO_{1-x}F_xFeAs$),where Rn=La,Ce,Sm,Pr,Nd.etc) having layered-structure like cuprates,has triggered challenge towards understanding the paring mechanism. In this work we analyze superconductivity and the Jahn Teller effect in this newly discovered $La(O_{1-x}F_x)FeAs$ superconductor. after reviewing the current finding on this systems, we suggested in phonon-mediated and distortion-field-mediated paring processes give the right order of superconducting critical temperature Tc.The distortion-field modes arise from Jahn-Teller effects due to degenerate or near-degenerate iron $3d_{xz}$ and $3d_{yz}$ orbitals.

The interaction of these degenerate electrons with phonon and distortion field results change of shape of orbitals consequentially a change in splitting of electronic orbitals. According to our calculated result in chapter three that superconducting parameters;energy gap (Δ) no of particles inside Fermi surface(N(0)),coefficient of isotopic constant (α) are affected due to Jahn-Teller distortion,consequently superconducting transition temperature (Tc) is affected . The calculated parameters are coincide with experimental values for suitable values of constants.

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Above all, I would like to thank the almighty; God, for letting me accomplish this stage.I am deeply indebted professor Singh my advisor, for his many suggestions and constant support and friendly approach during this research. His tireless follow up and his consistent support will be in my memory forever. My strongest thank is addressed to my Family and my intimate Friends, who lived for myself. They are the hero of my success with out their push and support, this stage is unthinkable. I have derived materials from many research and recent journals and books, and I am indebted to the authors of those publications and books.

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Introduction

Superconductivity was discovered in 1911 by H. kammerling Onnes in Holland while studying the electirical resistivity of a sample of frozeen mercury (Hg) as function of temprature. He found that the electrical resistance of pure mercury (Hg) droped abruptly to zero upon cooling to below (4.2K). He concluded that mercury (Hg) has passed into new state and gave the name superconductivity. To this new phenomena, the temperature below which a sample is superconducting in the absence of magenatic field is known as critical temperature (T_c). At any given temperature $T < T_c$,there is certain minimum field ($\bar{\mathrm{B}}$c(T)),called the critical field. Following onnes discovery ,many other materials ,alloys and complex ceramics were investigated in serach of superconductivity. After this, many other properties of superconductivity were discovered. It has been shown by Meissner and Oschsenfeld ,that superconductor is not only perfect conductor, but also perfect diamagnet [2]. Besides to this after series of experiments Bardeen ,cooper and shrieffer developed a theory about superconductivity so called "BCS" theory and they recive nobel prize in 19 72 .There mechanism of superconductivity is mediated by phonon as limitation superconducting transition temperature (T_c) is less than 30K. However, workers in this field Bednortz and Muller in 19 86 working in an IBM laboratory in swizerland found superconducting transition temperature (T_c) of new cuprate family up to 92K were discovered. Only five years after bednurz and Muller publication of (T_c) of superconducting cuprate family ,superconductivity in alkali metal doped fullerens have been discovered with transition temperatures as high as 33K in $RbCs_2C_{60}$ at anmbliet pressure, the highest (Tc =40K). Numerous experimental investigations of these superconductors shows

unique properties and Distinguish them from other superconductors , due to system is being completely new class of superconductors [9]. In addition to this,the discovery of superconductivity in LaOFeAs family of compounds is really exciting. Very soon after the discovery of up to 26 K superconductivity in $La(O_{1-x}F_x)FeAs$
(T c = 41 K) in $Ce(O_{1-x}F_x)FeAs$,(T c = 52 K) in $Pr(O_{1-x}F_x)FeAs$, and (T c = 55 K) in $Sm(O_{1-x}F_x)FeAs$ were reported. More and more experimental and theoretical studies suggested that the superconductivity found here is unconventional non BCS type. Several possible pairing mechanisms have been discussed theoretically and experimentally [42].

Chapter 1

GENERAL INTERODUCTION TO SUPERCONDUCTIVITY

1.1 BCS theory for conivenational superconductors

Since 1957 the undelying microscopic theory of super conductivity in metals was unveiled by J.Bardeen, L.N cooper and J.R schrieffer,which is named as BCS theory. In normal metals,the situation is well described by free electrons behave as free particles and the metalic ions play a limitted role in superconductivity. BCS theory outlines how in the presnce and attraction between electons of (cooper pairs) the normal state of other wise free electron gas becomes unstable to the formation of coherent many-body ground state.The mechanism of behind the weak attractive force binding the cooper pairs was actually first suggested by Herbert Frolich. He proposed that the same mechanism responsible for much of the electrical resistivity in metals (i.e the intraction of conduction electrons with lattice viberations) leads to electron-phonon interaction was born out of experiments which found that the critical temperature Tc varied with isotopic mass ,in simple terms, an electron interactions with the lattice by virtue of the coulomb attraction if feels for the metallic ions ,the results is deformation of lattice (i.e results phonon). A second electron in in the vicinity of deformed lattice corresponding loweres its energy , resulting is an electron -electron attraction via a phonon,viewed in this context as shown

below Fig(1.1),the superconducting order parameter $\psi(r)$ from GL theory can be interpreted as one particle wave function describing the position of the center of mass of cooper pairs[5]. Desipite being an extremely weak attraction bound pairs from in part because of the presence of Fermi sea of additional electrons ,as result of the Pauli exclusion principle , electrons that would prefect to be in state of lower kinetic energy can't populate by other electrons,thus a Fermi sea is requires to ensure the formation of all cooper pairs. The force of attraction between electrons which comprise a cooper pair has a range equivalent to the coherence length [1]. One of the most remarkable features emerging from BCS theory is the existence of an energy gap $\Delta(T)$ between the BCS ground state and the first excited state [2]. The BCS theory estimates the zero temperature energy gap $\Delta(0)$ as follow [15].

$$\Delta(0) = 1.76 K_B Tc. \tag{1.1.1}$$

and the nearest critical temperature Tc [3].

$$\frac{\Delta(T)}{\Delta(0)} = 1.74(1 - Tc/T)^{\frac{1}{2}}. \tag{1.1.2}$$

The energy gap is approches zero continuously as $T \longrightarrow Tc$. At low temperatures the energy gap is virtually independent of temperature and much larger than the enerergy $K_B T$. The probability of exciting a single electrons with energy E_k is then propertional to Boltzman factor

$$exp(-\frac{E_k}{K_B T}) \tag{1.1.3}$$

The maximum value of this probability is the exponential to shows experimental decrease at low temperatures [6].

So that different expression were given to superconducting parameters and let us see few for transition temperature,(T_c)

BCS's expression

$$T_c K_B = 1.14 \omega exp(\frac{-1}{NV}). \tag{1.1.4}$$

Mc Millan equation

$$T_c = \frac{\omega}{1.2} exp[\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}]. \tag{1.1.5}$$

Bogoliubov model gives

$$T_c \propto \omega_d ex(\frac{-1}{\lambda - \mu}). \tag{1.1.6}$$

1.2 Cooper pairs

The behavior of superconductors suggests that electron pairs are coupling over a range of hundreds of nanometers, three orders of magnitude larger than the lattice spacing Called Cooper pairs. These coupled electrons can take the character of a boson and condense into

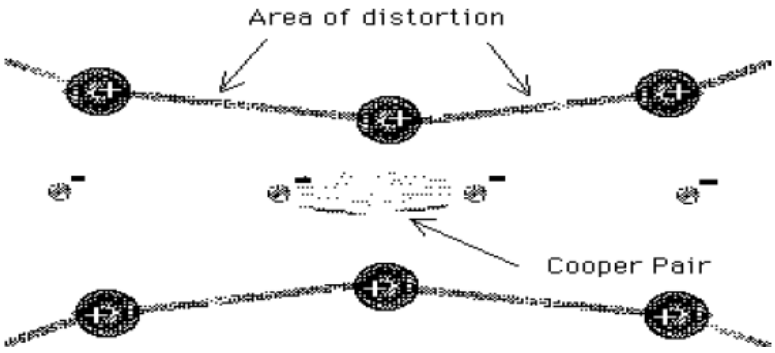

Figure 1.1: A schematic representation of cooper parirs

the ground state. The effective net attraction between the normally repulsive electrons produces a pair binding energy on the order of milli-electron volts, enough to keep them paired at extremely at low temperature. The transition of a metal from the normal to the superconducting state has the nature of a condensation of the electrons into a state which leaves a band gap above them. The boson-like behavior of such electron pairs was further investigated by Cooper and they are called "Cooper pairs".

1.3 An alternative to BCS theory

There were early doubts about the validity of BCS theory because its prof of meissner effect failed to stasify gauge invariance.However ,it was later shown that the BCS derivation was valid in the pariticular case of to an arbitrary gauge a points of BCS theory to an arbitrary gauge a part of BCS theory are certainly correct and represented an important adivance when frist proposed; the concepts of cooper pairs, of macroscopic phase coherence and the existence of an energy gap are incontrovertible.These elements of theory leads to explanation and even prediction of puzzeling experimental data such as Josephon tunneling . However, many other aspects of BCS theory and especially the electron-phonon mechanism are not correct despite being universally accepted. For the past 20 years, workers of in this field have been developing an alterinative to BCS theory it applies to all superconductors inculding hole superconductivity.

The essential aspect of the theory stated as below;[4].

1.Electron-hole asymmetry is key to superconductivity;hole carries in normal state are necessary for superconductivity,

2.Electron-phonon interaction does not cause superconductivity;Superconductivity is driven by a purely electronic mechanism and is associated with kinetic energy lowering.

3.Material characteristics favorable for high T_c are transport in the normal state dominated by hole carries and excess negative charge the substructures(i.e plane) where conduction occurs, superconductors expel negative charge from their interior toward the surface in transition to superconductivity.

4.The spin-orbit interaction play a fundamental role in superconductivity.

Those are some of essenial elements has been BCS theory failed to answer [5].

1.4 Meissner effect

Superconductors exhibit unique behavior. This was first observed by H.W Meissner and R.Oschenfeld In 19 33,they found that if a superconducter is cooled in a magnetic field to below the transitions temperature,the transitions lines of induction $\vec{B}$ are pushed out as shown below Fig (1.2) .

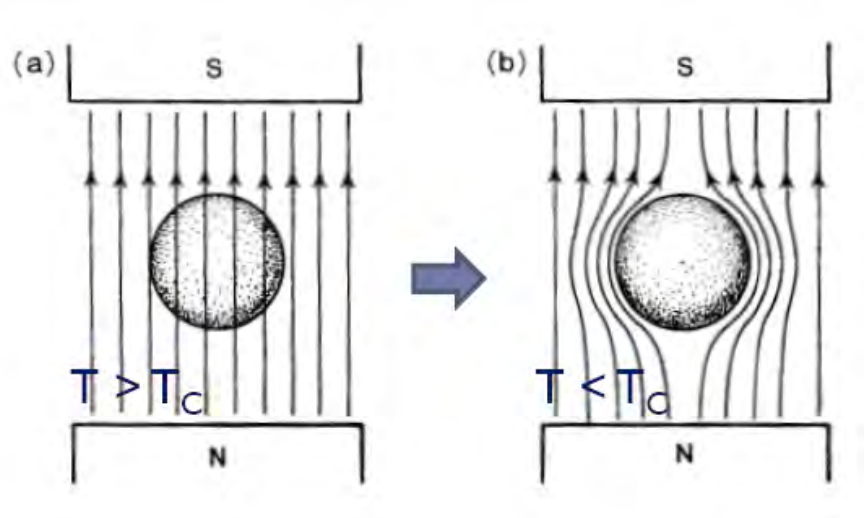

Figure 1.2: A schematic representation of Image of magnetic field lines and a superconductor

The meissner effect shows that a bluk superconductor behaves as if inside the specimen ($\vec{B} = 0$).

Becauuse of farady's law,the magnetic field inside a superconductor canot change because there is no emf due to the lack of electric resistance thus to prevent this,a current is induced in the superconductor which cancels out as shown below Fig (1.2) that a image of the magnetic lines and a superconductors.

1.4.1 London equation

The mathematics of meissner effec was described by London equations.The following equation were developed to explain the behavior exhibited Meissner effect quantitatively[2].

Suppose that an electric field momentarily arises within a superconductor. The superconducting electrons will be freely accelerated with out dissipation so that their mean velocity $\vec{v}$ will satisfy the equation number (1.4.1)

$$m\frac{d\vec{v}}{dt} = -e\vec{E}. \tag{1.4.1}$$

Since the current density carried by these electrons is

$$\vec{J} = ev_s n_s. \tag{1.4.2}$$

equation (1.4.1)can be written as

$$\frac{d\vec{J}}{dt} = -\frac{n_s e^2 \vec{E}}{m}, \tag{1.4.3}$$

but from Maxwell equation

$$\nabla X\vec{E} = \frac{-1}{c}\frac{\partial \vec{B}}{\partial t}, \tag{1.4.4}$$

$$\nabla X\vec{B} = \frac{4\pi}{c}\vec{J}. \tag{1.4.5}$$

upon substitution of(1.4.5) into (1.4.3) And taking curl both sides of equation

$$\frac{c}{4\pi}\frac{\partial}{\partial t}(\bigtriangledown \times \bigtriangledown \times \vec{B}) = -\frac{n_s e^2(\bigtriangledown \times E)}{m} \tag{1.4.6}$$

$$\bigtriangledown \times \bigtriangledown \times \vec{B} = \bigtriangledown(\bigtriangledown.\vec{B}) - \bigtriangledown^2\vec{B} \tag{1.4.7}$$

An account of (1.4.4) togther with (1.4.7) results

$$\nabla^2\vec{B} = \frac{4\pi n_s e^2}{mc^2}\vec{B}. \tag{1.4.8}$$

In similar way one can calculate for curent density ($\vec{J}$)

$$\nabla^2\vec{J} = \frac{4\pi n_s e^2}{mc^2}\vec{J}.. \tag{1.4.9}$$

$$\nabla^2\vec{B} = \frac{\vec{B}}{\lambda} \tag{1.4.10}$$

Where

$$\lambda = (\frac{mc^2}{4\pi n_s e^2})^{\frac{1}{2}}. \tag{1.4.11}$$

Hence equation (1.4. 10) is known as the London equation which is independent of time; The soluation for equation no (10) when a magnetic field perpendicular to at a given depth of the surface λ is .

$$\vec{B}_z(x) = \vec{B}_0 e^{\frac{-x}{\lambda}}. \tag{1.4.12}$$

This equations in turn, predicts currents and magnetic field in superconductors can exist only within a layer of thicknes λ of the surface and magnetic field decay in superconductor exponentialy; where λ is known as the london penetration depth [2,43].

1.4.2 TypeI and typeII superconductors

An important difference in typeI and typeII superconductor is in the mean free path of conduction electrons in the normal state[43]. If the coherence length(ξ) is longer than london penetration depth (λ) ,the superconductor Will be typeI ,most pure metals are typeI with $k < 1$. But ,when the mean free path is short,the coherence length is short and the penetration depth is greater. This situation when ($k = \frac{\lambda}{\zeta} > 1$) and the superconductor will be typeII [43].

1.5 High temperature superconducters(HTS)

Ever since superconductivity was discovered by Kammerling-Onnes in 1911, there has been continuing efforts to find a new superconductors with higher transition temperatures[8].Decades of efforts and rather slow progress culminated in the discovery of high Tc superconductivity in $La_2xBaxCuO4$ by Bednorz and Muller in 1986[6]. The modification of the original oxides by introducing the smaller Y^{+3} for orginal L_a^{+3} results in a gaint jump of Tc to 92K [7].More recently a new members of cuprate family has been synthesized .One of them reaching a $Tc \sim 163K$ Tl-based cuprate under pressure were discovered [6], which is six times larger than the previous world record of $Tc \sim 23K$ in Nb3Ge shook the foundation of phonon-mediated pairing mechanism. Besides high temperature superconductivity in cuperate oxide ,the superconductivity

alkali doped A_xC_{60} persisting up to very high temperatures ($T_c = 33K$) has been discovered[8].The discovery was rised important question about superconductivity in low-band width molecular sollids [9]. Zhang etal estimated various contribution to the electron-electron interaction in K_3C_{60} and argued that the K^+ optical phonon modes induces strong attraction, which is the main source of superconductivity [10]. A suggestion by Lanno etal ,is that dynamic Jahn Teller coupling involving high frequency intermolecular vibrations strongly scatter electrons near the Fermi surface leading to superconductivity in addition to phonon-mediated electron paring mechanisms in this system. Chakran and Tosatti argued that two electrons may pair by electron-electron exchange and correlation on a single C_{60} molecule [11]. As shown below (figure 1.3) BCS theory based on electron phonon intraction is not capable of explaning such high T_c values in a cup rates and alkali metals doped c_{60} superconductors. Hence,a number of theories have been proposed by a several workers which involve phonons,excitons bi-excitations polrons ,spinflu actions etc....to explain superconductivity in high transition temperature and other unusual properties of these systems [12]. Discovery of a new superconductor always attracts strong attention of the scientific community particularly if the critical temperature (Tc) is above 20 K. Following the discovery of the first high-transition temperature superconductivity in copper based compounds two decades ago,a second class of high-transition temperature superconductors has been recently reported in iron pnictides in the transition temperature T_c as high as 56K were discovered.This discovery of the iron-based layered superconductor ($LaFeAO_{1-x}F_x$) was frist time reported by kamihara etal on February(2008) has great impact to researchers in condensed -matter physics.So far intensive experimental and theoretical efferts have been devoted to understand the nature of the superconductivity uner this phenomenon [13]. It is rather surprising that imediately after the recent news of superconductivity of ($LaO_{1-x}FxFeAs$) several papers, both theoretical and experimental,have been circulated in the community. There may be four main reasons why this discovery has produced

such a strong impact.

1.(Tc) is relatively high (26K)

2. It is a new finding that Fe,which is a typical magnetic element, seems to be participating to superconductivity.

3. The crystal takes again a layered structure and the doping region and the superconducting region are geometrically and electronically separated.

4. The material seems to have strong flexibility in the choice of constituent elements (suggesting posibility of higher Tc materials in the same category).

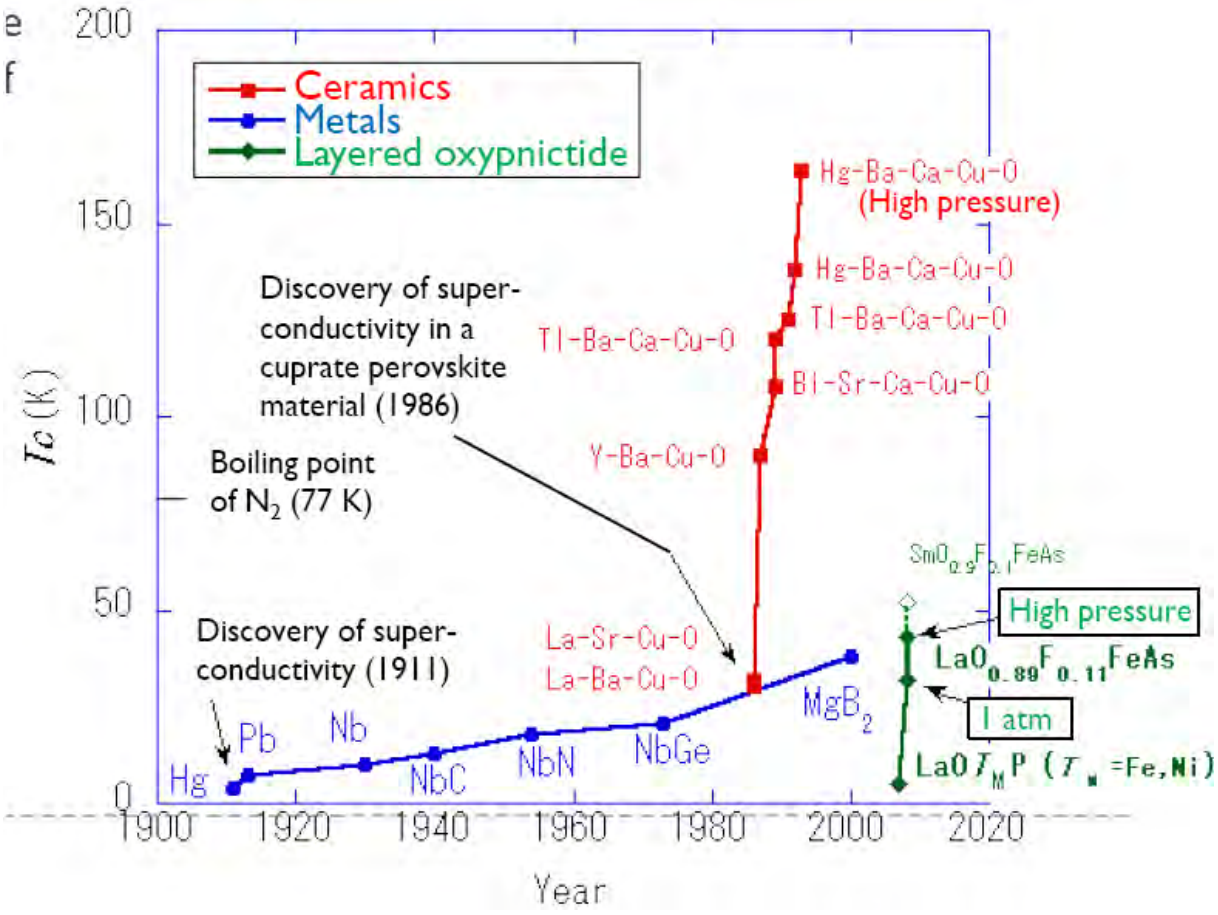

Figure 1.3: A schematic representation the development of superconductivity over the year

Chapter 2

REVIEW ON SUPERCONDUCTIVITY AND JAHN TELLER EFFECT IN $LaO_{1-x}F_xFeAs$ SUPERCONDUCTOR

2.1 Brief introduction to Jahn-Teller effect(JTE)

The Jahn-Teller effect (interaction) which is an example of electron-phonon interaction was first time seen by Jahn and Teller in 19 34. The name Jahn-Teller effect(JTE),which include the proper(JTE),pseudo(JTE),and Renner Teller effect. Now days forms a whole trend in the theory of the structure and properties of molecules and crystals jointly termed as John Teller vibrionic coupling effects or abbreviated(JTE).It is an approach to (a tool for) general understanding and solving of molecular problems, which is in principle applicable to any system more than two atom [14,42]. As far many other fundamental properties of matter, the(JTE) was first formulated in the early thirties of the twentieth century there were four persons who initiated this trend,L.Landu, E-Teller,H.Jahon ,and R.Renner in 1934. L.D Landau was discussed with E.Teller about his student's (R.Renner's) work and first time formulated the statement that a molecule in an orbital degenerate electronic state is unstable with respect to spontaneous distortion of nuclear

configuration that removes the degeneracy[16]. In 1950 Abragam and price first revealed the dynamic nature of the JT distortion by analyzing the temperature dependence of ESR spectra of Cu(II) disappeared at the certain temperatures due to thermal averaging over different direction of JT distortion[32]. The (PJTE) probelms was formluated for frist time the idea behind the PJTE is that not only exact degeneracy (required by the JT theorem),but sufficiently (close-in-energy pseudo degenerate) states may produce instabilities similar to those of (JTE). The condition of PJTE instability requires that the energy gap between the mixing state is sufficiently small in comparison with other vibrionic parameters of the system. The (PJTE) become most important later when it was shown that it is the only source of instability of high-symmetry configuration of polyatomic systems in non degenerate states. Qualitatively (roughly) the origin of instability of molecules in high-symmetry configuration with orbital degeneracy can be easy understood if one takes into account that when there are more electronic distributions with the same energy, they are necessarily non totally symmetric with regard to the environment. For instance the three atomic p states, P_x,P_y and P_z and Hence the electron on any of them distorts the other wise symmetrical environment, thus lowering its energy [16]. An important development of JTE theorem began with the treatment of interaction of JT centers, especially regular JT centers in crystals, known as the cooperative JTE(CJTE) kanamori in 1960 first explicitly explored such cooperative phenomena in JT crystals. In 1966 Bersuker first suggested the vibrionic theory of ferroelectricity as a cooperative PJTE. During the 1980's alongside applications of the JTE to physical and chemical phenomena, a new development of the theory emerged first and numerical calculation of vibrionic coupling effects become more widespread . Among chemical application attention was paid to the JTE in stereo chemistry and chemical activation and in mixed-valence compounds. In general about the theory more attention has been also paid to multi-model problems quite and a number of papers in 1970's and 1980's were developed to JTE in impurity centers in crystals. At this point the geography of JT symposium become more wide speared and theory

attracted more participates and different symposium took place in different cantries and international workshop was organized in Beijing since 2004 [16].The Jahn-teller(JT) theorem was well known in the chemistry of complex units non linear molecule or a molecular copllex exhibiting an electronic degeneracy will spontaneously distort to remove or reduce this degeneracy. A complexes containing specific transition metal(TM) central ion with special valency show this effect[7]. In the linear chain model(Hock et al) 1983,for small JE distortion with stabilization energy E_{JT} smaller than the band widith of metal only slight perturbation of the traveling electrons in present with increasing E_{JT} ,the tendency to localization is enhanced ,and for E_{JT} being of the magnitude of the band width . These composites of an electron and a surrounding lattice distortion with high effective mass travel through the lattice as whole and a strong electron phonon coupling exists oxides containing (TM) ions with partially filed e_g orbitals , like Ni^{3+},Fe^{4+} or Cu^{+2} exhibit a strong(JTE) and we considered these as possible candidates for new superconductors [7]. An illustration of the JT aproach to electron-phonon coupling in solids may be found in modern attempts to explain the Origin of high temperature superconductivity (HTSC)[7]. The question remains whether the Jahn-Teller effect play any role in high T_C superconductivity beyond

that of producing the static distortion of the CuO_6 octahedral for cuperates case. Many of the earliest efforts have been devoted to explaining high T_c superconductivity involved exotic magnetic interactions. However, recent experimental and th theoretical researches have been revealed a strong connection between phonon states and superconducting in cu-O compounds in particular Araietal have recently pointed out that anomaly in phonon states in short-range region,associated with a local structeral distortion is a common

feature of high (T_c) oxide superconductors at T_C given these indication, it is reasonable to consider the possible ways in which the Jahn Teller effect might influence supper conductive paring. A number of researches have been proposed model in which Jahn Teller interactions give to rise superconductive

paring. Among those A Reversed paring model and d-d excitation model are some of examples[32]. Besides to high temperature superconductivity and instability in cuperates the recent discovery of soccer-ball shapped C_{60} molecule and the susequent realization that solid C_{60} could become superconducting when doped whith Alkali metal (K,Rb Cs). The geometry of the C_{60} molecule,which is centeral to the properties of these compounds (the fullerides). In its ground state it is neutral C_{60} posses a closed shell electronic structure and thus no Jahn-Teller interaction is expected. However, because the lowest uncocupied molecular orbital(LUMO) is three fold degenerate,a jahn teller interaction will be possible when C_{60} is excited to this oribital and for anions such as C_{60}^{-}, C_{60}^{3-} (the charge state in alkali doped solids such as Rb_3C_{60}[17].According to recent study, The Jahn-Teller effect is caused by the interaction of a degenerate electronic state with molecular vibrations. In C_{60} anions, the electronic states involved are those of the triply degenerate t_{1u} orbitals and the vibrations are the ten fivefold degenerate (Hg) modes.These interactions result in a change of shape of the molecule and consequently a change in the splitting of the electronic orbitals. Electrons will occupy the lowest-energy levels and thus, if the splitting is large enough, overcome Hunds rule and form non magnetic systems. on the other hand JT distortion is forcing an icosahedral C_{60} molecule into a crystal inevitably lowers its symmetry[17].

2.2 Structure and electronic property $(LaO_{1-x}F_xFeAs)$

Clearly understanding the electronic, magnetic and structural properties of the parent compound LaOFeAs(when x=0) is key to determining the underlying mechanism that makes these materials superconduct upon electron (hole) doping. It has been reported that from experimentally,all iron-pnctide superconductors inculde a two dimensional (2-D) FePn (Pn; pnitrogen atom) layers with a tetragonal structure at room temperature as shown below (Fig 2.1). Therefore, at glance their physical properties are considered to be highly two dimensional. The first discovered iron-pnctides superconductor

$laO_{1-X}F_xFeAs$ has space group $P4/nmm$ with cell parameters of ($a = b = 4.0355A^0$,$c = 8.7393A^0$) [18,19]. In this newely discovered copound supersingly spectral weight close

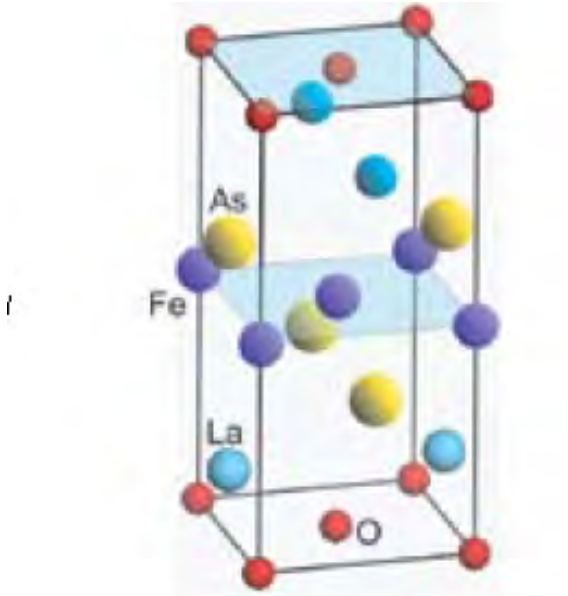

Figure 2.1: lattice structure of LaOFeAs

to the Fermi energy are contributed by the Fe 3d orbitals. As the Fe is the only ion in the system that posses a unclosede shell. Thus,a microscopic model for the system can be very complicated. Since all five of the Fe 3d orbitals is involved. In principle, a relevant microscopic model,besides being as generic as possible,should frist account for peculiarities of the undoped pnictide ;the system is is neither a good bad metal,through it has a unclosed 3d-shell,nor a good band insulator,through it has an even number of electrons per site [20]. Interestingly the system (LaOFeAs) is sensative to F dooping. F -dopped LaOFeAs and its derivates with rare earth substitution arose many interests in community of condesed matter. It is superconductor with transition temperature ($T_c \sim 26K$). Similar to the high T_c cuprates, the iron-based superconductors also have a layered structure in which the role of the copper oxgen plane in the high T_c cuprates is played by the FeAs plane.

At the same time,both systems showes similar phase diagram with antiferromagnetic ordered phase and superconducing phase next to each other.Dspite these similarities,the

cuprates and pnictides have some important differences[19]. Fristly the undoped iron oxypnictides with SDW order are poor but metalic conductors,rather than the Neel antiferromagnetic insulators in undoped and compliacated Fermi surface(FS).Significantly different from the situation in cuprates, and the nature of superconductivity of iron pnictides and cuprate are profoundly different [20] to date, frist principles electronic structure calculation have shown that, in iron pnictides Fe 3d orbits contribuite the major special weight close to the Fermi energy and the Fermi surface (FS) of LaOFeAs consists of two hole type-circles around the Γ point and two electrons type centered ellipses around the M point as shown below (Fig 2.2). The origin of superconductivity in the doped pnictides has been hotly debated several groups and it it has been examined by the band structure as calculated from density functional theory (DFT) [26]. On the other hand pecularities on the system stated by relivant microscopic model was magnetic ordering. on the squre lattice, a magnetic order is at $(\pi, 0)$ is quite unusual and it reveals us to the system showes metallic rather than insulating behavior in magnetic ordered state.More over,the magnetic ordered phase is next superconducting phase,it is natural to expect the magnetic correlation to a play a key rule in the origion. Some people tried to formulate a phenomenological theory based on the results of the existence of small electron poket and small hole poket found in DFT calculations and there nesting play a key role to account for transpot and magnetic properties of the parent copounds(LaOFeAs)[20]. Due to above and other cases undoped system is by accident very close to semi-metal and the instability caused by nesting between the small electron poket and small hole pocket gives to rise to the magnetic ordered at $(\pi, 0)$. The presence of nesting of electron and hole inside Fermi surface in extended zone (2 hole paket Γ ,electron pokets on edges) is play a great rule in this system,it coposed of d orbitals nesting for (π, o) SDW and popular two bands, namely d_{yz} and d_{xz} has hole wrong postion at x=0, prefect electron hole nesting at $(\pi, 0)$, if t=0 we expect fully gaped SDW.were t is nesting betwheen[21,42]. On other hand,the concept of nesting becomes totally irrelevant to account for a ordered moment as large as

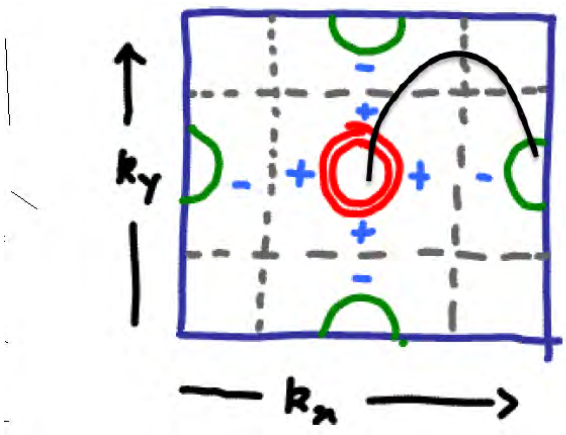

Figure 2.2: Nesting between electron and hole inside Fermi level

one μ_B according to the density functionality calculation. In this newly discovered superconductors,the most intriguing issues was pairing mechanism and pairing symmetry.To date various possibilities of superconducting mechanism and pairing symmetry in iron-based superconductor have been proposed theoretically and experimentally.Theoretically, proposed superconducting pairing symmetries range from spin singlet d-wave,s-wave or mixtures of the $Sx^2 - y^2$ wave and $d_{x^2-y^2}$ to spin triplet p-wave.Experimentally, the nature of the superconducting gap observed is also very different from author to author and from sample to sample [22]. However,based on symmetry consideration,it has been proposed that extended s-wave pairing for superconducting state[21]. On the other hands, it has been proposed that superconductivity in LaOFeAs probably non-phononic in origin[23].

2.3 The effect of fluorine doping on oxypnictide

The recent experimental and theoretical study of the $LaO_{1-x}F_xFeAs$ compounds with and without fluorine doping by density functional calculation reveals as F doping has a significant effect.When paying attention to the behavior of the charge. The substitution for the O sites with F changes the bond length and angle in distorted LaO tetrahedron where as weaker geometric effects were observed in FeAs layer, further F doping induces large decreases in the c-axis length and the La-As distance suggesting an enhancement of

the charge polarization in the $(LaO)^{\delta+}$ and (FeAs) $^{\delta-}$ layers as result of electron transfer between two layers. On other hand,F-doping reduces the a and b axes length by certain amount at room temperature. The reduction of a-axis length indicates the decrease of Fe-Fe distance which enhance the interaction among 3d electrons (increase fluctuation). Thus doped (LaOFFeAs) is superconducting with superconducting transition temperature experimental value (T_c)=26K [24]. More over it has been found experimentally, with increasing fluorine doping the structural phase transition decreases gradually dome near(x=0.10),where as the ferromagnetic order is suppressed before the temperance of superconductivity and also the long range static AFM order is suppressed on electron doping to induce superconductivity[25]. The other main effect of Electron doping by F is an efficient way to suppress the nesting effect (the SDW instability), because the shifting of Fermi level enhances the mismatch between electron and hole FS. In addition to this,suppression of phase transition by F doping reveals us to,F doping enhance degeneracy which also enhance T_c according to reference [42]. The other effect of fluorine in the electronic structure O foxypnictide is to change the orbital symmetry at Fermi level distribution dominated by $3d_{z^2}$ unperturbed charge distribution for non super conductive LaOFeAs. However as some oxygen atoms are replaced with fluorine the symmetry inside the perturbed crystalline field change to somethings akin to $d_{x^2-y^2}$ orbital. The orbitals in $d_{x^2-y^2}$ inside tetrahedral field allow a better electronic interchange than the d_{z^2} orbital [26]. The effect of F doping to LaOFeAs summarized as:

1.The F-doping acts as electron donor,leading to extra electrons to the FeAs layers which results in shift of the chemical potential to lower binding energy side

2. The c-axis length and LaAs distance are shortened as result of the enhancement of the charge polarizations of the $(LaO)^{\delta+}$ and $(FeAs)^{\delta-}$ layers.

3. The Fe-Fe distance decreases,which may enhance the interaction among 3d electrons

4.The distortion of the LaO tetrahedron is relaxed largely,where as less structural changes take place in FeAs tetrahedron. It is likely that interplay of these effects may prohibit

the crystallographic and magnetic transition to occur and generate the superconducting phase[27].

2.4 Structural phase transition and Jahn-Teller effect (JTE)in $(LaO_{1-x}F_xFeAs)$

Cruz.etal.reported that from netron-scattering experiments that, the physical properties of resistive anomaly in LaOFeAs. The structural phse transitions at $T_s \sim 150K$ in LaOFeAs,this result demonstrates that LaOFeAs undergoes an aprupt structural distortion below 155K and the symmetry changes from tetragonal(space group P_4/nmm to Orthorhombic (space group). Also it has been noted that the presence of lattice distortion above the Neel temperature (T_N) and lattice distortion is apparent at 138K. Therefore, the resistive anomaly at approximately 150K is caused by structural distortion. Incontestably ,neither structural nor magnetic anomaly was observed in superconducting $La(O_{0.92}F_{0.08})FeAs$. More over,the experiment revels to us magnetic ordering is highly related to structural distortion [14]. The origin of this anomaly has been recently determined by neutron scattering studies. In adition to this,from density functional theory analysis shows that lattice constant of undoped sample the a-axis length starts to split at $\sim 160K$ (structural phase transition) and magnetic transition temperature at 140K [28]. According to recent experimental result LaOFeAs exhibits spin-density-wave (SDW) and antiferromagnetic long-range ordering with a small moment (0.35 μ_B per Fe) followed by a small structural distortion .On the other hands,the cause of this SDW ordering has been predicted from Fermi surface nesting of 3d orbitals [26]. More over ,the density functional calculation reveales as ;the nearest and nexst nearest neighbor superexchange interaction between the iron(Fe) ions in LaOFeAS are large,antiferromagnetic(AF),gives to rise a frustrated magnetic ground state which consists of two interpenerating AF square sublattices with M(Fe)=48μ_B the system lowersits energy further by removing the frustration via

a structural distortion. In general it has been studieed that different antiferromagnetic structure on the system which reduces the symmetry of crystal from tetragonal to orthorhombic.These magnetic structures look strage at frist sight but the angular vibration of d orbitals can adjust the covalency between Fe atoms to be consistent with magnetic structures accomplished with orbital ordering and crystal structure with orbital ordering.But crystal structure is consistently modified from the tetragonal symmetry, which leads as to generalization modification of crystal structure mediated by orbital ordering [24].In addition to this, density functionality theory analysis showon from below figure schematically the potentioal energy surface (PESs) calculated for the spin stripe type configuration (AF2) of the Fe electron spins in undoped LaOFeAs as a function of the difference between the orthorhombic a and b axis length (d), AF2 PES is represented by two equivalent parabolic curves with the minimum at the certain ($\pm d$) values in the $a < b$ and $a > b$ regions. The lower branch has the double minimum structure and the state is stabilized at one of the minima, this indicates that the orthorhombic phase is stable at low temperatures (static Jahn-Teller effect) with increasing temperature ,the state migrates dynamically between the two minima because of the termal energy inducing transition from orthorhombic to tetragonal phase (dynamic Jahn-Teller effect).Where T and O represent tetragonal and orthorhombic phases,respectively. Spin configurations for AF2a and AF2b in both $a > b$ and $a < b$ are shown below figure. The calculated double minma most likely arises from both existence of the energy degenerate d orbital states near the Fermi surface level and magneto restriction interaction between the Fe spins, which is known as Cooperative Jahn-Teller effect. With increasing electron density by the F-doping he chemical potential shifts to a lower binding energy and magnetic moments Decreases . These leads to no energy gain by Jahn-Teller distortion,resulting in suppression of the phase transition this anlaysis leads to generalization undoped LaFeAsO undergoes a crystallographic phase transition from tetragonal P_4/nm to orthorhombic (cmma)at $\sim$140K, the transition are likely caused cooperative Jahn-Teller effect.

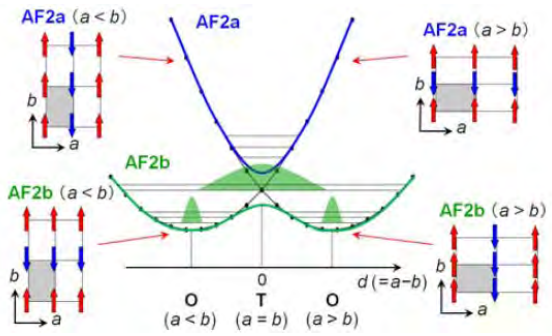

Figure 2.3: Schematic potential energy surfaces of two kinds of stripe configurations, AF2a and AF2b in undoped LaOFeAs

.

Moreover,the sturactural distortion deponds on bond angle between Fe-As-Fe.

we note that for $\gamma = 90^0$, the orbitals d_{xz} and d_{yz} are degenerate and we have original teteragonal cell .However, once angle between Fe ions (γ) deviatesfrom(90) (a and b axes are no longer equal) the sturacture change to orthorhombic and digenerence between the orbitals are resolved this leads to as the system is subjected to symmetry lowering Jahn-Teller effect. In addition to this, theoretical proposed model to explain the phenomena existing distortion of LaOFeAs is effective two-band tight binding model for the low energy physics of the FeAs plane. The two bands,which have been derived from the two degenerate Fe 3d orbitals $3d_{xz}$ and $3d_{yz}$ enjoy the largest itineracy among all the five Fe. 3d bands as a result of hybridization with As 4p orbitals. Also it explains naturally the largest geometrical frustration which is necessary for the formation of the magnetic order with wave vector$(\pi, 0)$ as found experiments . The hopping bridged by the As 4p orbitals is peculiar in that a anistopic. This anisotropy in kinetic energy provides an interesting way to break the degeneracy between the $3d_{xz}$ and $3d_{yz}$ bands and lower the symmetry of the system from tetragonal to orthorhombic spontaneously via a kinetic energy driven by Jahn -Teller processes [20]. In principle, all the five Fe 3d orbitals are equally important for the low energy physics in the presence of crystal field ,the five fold degenerate Fe 3d atomic orbitals will split according to the irreducibly representation of the crystal symmetry. As the same time,the bands drived from the Fe five 3d orbitals have

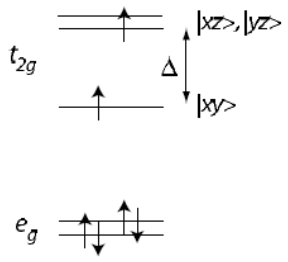

Figure 2.4: Schematic representation of Fe 3d oribitals

quite different kinetic energy.The $3d_{xz}$ and $3d_{yz}$ bands enjoy the largest itineracy among the five Fe bands as mentioned above reason. The remaing three orbitals;namely,$3d_{xy}$, $3d_{z^2-r^2}$ and $3d_{x^2y^2}$ are more localized as their hybridization with the As 4p orbitals is much less effective. Here we assume the crystal field splitting and the orbital selective hopping effect to be sufficiently strong to retain only the $3d_{xz}$ and $3d_{yz}$ orbitals for the discussion of the low energy physics. We note in advance that the bands derived from

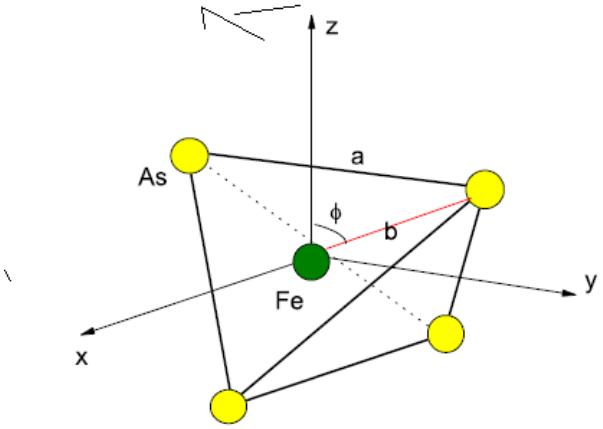

Figure 2.5: The squeshed tetrahedron formed by the four neighboring As ions around each Fe ions in the plane FeAs in undoped LaOFeAs

3dxz and 3dyz orbitals have much larger itineracy as compared to that $3d_{x^2-y^2}$ orbital as a result of the indirect hopping bridged by As. With this simplification, we left with a model with two degenerate bands, 3dxz and 3dyz. In this model,each Fe has three 4p As orbitals in its outermost shell. Since the $4p_z$ orbital is far away from the Fermi energy,we consider only the hopping path mediated by the $4p_x$ and $4p_y$ orbitals of As ion.

As a result,the dispersion relation of the 3dxz (3dyz) band has an orthorhombic rather than tetragonal symmetry(the tetragonal symmetry of the system is recovered when both bands are taken into account). This anisotropy originates from other Fe 3d orbitals,as there electron clouds have the best chance to reach the As ions which site above (or below) the center of the Fe plaquete. Such a orbital selective hopping effect provides a natural explanation for the much larger itinerancy of the 3dxz and 3dyz bands as compared to other 3d bands found in DFT calculations.The degeneracy between $3d_{xz}$ and $3d_{yz}$ bands and its spontaneou s breaking through a kinetic energy driven Jahn-Teller process provide a natural way to understand the structural transition[20]. As it shown from (Fig 2.5) the orthorhombically distorted Fe plaquette, It is clear from the figure that with the lowering of the symmetry from being tetragonal to being orthorhombic.

2.5 The effect of structural distortion on electronic structure and magnetization

The recent experimental result performed by analyzing the electronic state before and after the structural distortion revealed that destortion have significant effect both on number of state at Fermi surface as well as the Fe magnetization. more over, it has been experimentally and theoretically stated that,the cause of structural distortion is antiferromagnetic frustration (AF2) [29]. Interestingly, the $N(E_F)$ is doubled while the magnetization is reduced by half due to structural distortion. The increase in the $N(E_F)$ shows that LAOFeAs exhibits metallic behavior after the transition Incontrast to cuprate, the destortion does not introduce any new active modes,But just splits the double - degenerate modes into non-degenerate once .However ,the splitting is quite small,the largest around 0.2meV. This explains why no new modes appear in optical measurements after transition [30].

Chapter 3

MATHEMATICAL CALCULATION OF SUPERCONDUCTING PARAMMETERS

Under this chapter we try to calculate superconducting parameters using the suitable formula and compare those calculated value with experimental value for this system(LaOFeFAs). Those parameters are;superconducting transition temperature (T_c),isotopic coefficient, (α) energy gap at zero temperature ($\Delta(0)$).It is believed fact that the cause of Jahn-Teller effect(JTE) for this system (laOFeAs) is due to interaction of d-orbital electrons (nesting electrons and hole inside Fermi surface).It is natural to expect more or less

phonon contribution to this system. Since the Jahn-Teller interaction is an example of electron- phonon coupling [32]. More over the structural distortion has effect of elongation or contraction of tetrahedron. On the other hands, it is believed fact that in general Jahn -Teller systems, including high transition temperature (T_c) superconductors, should be examined carefully for a direct or indirect role of phonons on the superconductor [33]. Therefore, phonon and its distortion frequency shall better to consider to explains the T_c values very well.

3.1 Derivation fOr superconducting transition temperature (Tc) From BCS Hamiltonian (H_{BCS})

The BCS Hamiltonin given by

$$H_{BCS} = \sum_{k,k'} \epsilon_k a^+_{k,\sigma} a_{k',\sigma} - \sum_{p,p'} V_{p,p'} a^+_{p\uparrow} a^+_{-p\downarrow} a_{p'} \downarrow a_{-p'\uparrow}. \tag{3.1.1}$$

The equation of motion for Green's function is
$\omega G(\omega) =< [\hat{A}(t), \hat{B}(t')] > + \ll [\hat{A}(t), \hat{H}], \hat{B}(t') \gg_\omega$.

Equation of motion for conduction electrons is given by

$$\omega G_{k,k'}(\omega) = \omega \ll a_{k\uparrow} a^+_{k\uparrow} \gg = \delta_{kk'} + \ll [a_{k\uparrow}, H_{BCS}]; a^+_{k\uparrow} \gg \tag{3.1.2}$$

Now putting equation (3.1.1) into (3.1.2) and evaluating

$$\omega G_{k,k'}(\omega) = \omega \ll a_{k\uparrow} a^+_{k\uparrow} \gg = \delta_{kk'} + \ll [a_{k\uparrow}, \sum_{k,k'} \varepsilon_p a^+_{p,\sigma} a_{p',\sigma} - \sum_{p,p'} V_{p,p'} a^+_{p\uparrow} a^+_{-p\downarrow} a_{p'} \downarrow a_{-p'\uparrow}; a^+_{k\uparrow} \gg \tag{3.1.3}$$

$$I_1 = \ll [a_{k\uparrow}, \sum_p \varepsilon_p a^+_{p\sigma'} a_{p'\sigma}] \gg \tag{3.1.4}$$

To solve above equation we evaluate the commution relation

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

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

$[A, BC]$ =$\{$A,B$\}$C$-B\{$A,C$\}$,

[AB,C]=$A\{B, C\}$-$\{A, C\}B$.

$$\begin{aligned} I_1 &= \{a_{k\uparrow}, \sum_p \varepsilon_p a^+_{p\sigma}\} a_{p'\sigma'} - \varepsilon_p a^+ \sigma \{a_{k\uparrow}, a_{p'\sigma'}\}, \\ &= \{a_{k\uparrow}, \sum_p \varepsilon_p a^+_{p\sigma}\} a_{p'\sigma'} \\ I_1 &= \varepsilon_k a_{k\uparrow}. \end{aligned} \tag{3.1.5}$$

$$I_2 = \ll [a_{k\uparrow}, -\sum_{pp'} V_{pp'} a^+_{p\uparrow} a^+_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow}] \gg . \tag{3.1.6}$$

this evaluated to give

$$I_2 = -V_k a^+_{-k\downarrow} a_{p'\downarrow} a_{-p'\uparrow}. \tag{3.1.7}$$

up on putting equation number (3.1.5) and (3.1.7) into equation of motion no (3.1.3)

$$\begin{aligned} &= \omega \ll a_{k\uparrow} a^+_{k\uparrow} \gg = 1 + \ll \varepsilon_k a_{k\uparrow}, -V_k a^+_{-k\downarrow} a_{p'\downarrow} a_{-p'\uparrow}, a^+_k \gg \\ &= 1 + \epsilon_k \ll a_{k\uparrow}, a^+_k \gg -V_{p'}, \ll a^+_{-k\downarrow} a_{p'\downarrow} a_{p'\uparrow} a^+_k \gg \qquad (3.1.8) \\ &= 1 + \epsilon_k \ll a_{k\uparrow}, a^+_k \gg -\Delta \ll, a^+_{-k\downarrow}, a^+_{k\uparrow} \gg, \qquad (3.1.9) \\ \Delta &= -\sum_{p'} V_p a_{p'\downarrow} a_{p'\uparrow}. \qquad (3.1.10) \\ \omega &\ll a_k \uparrow a^+_{k\uparrow} \gg = 1 + \varepsilon_k \ll a_{k\uparrow}, a^+_k \gg -\Delta \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg \qquad (3.1.11) \\ (\omega - \varepsilon_k) &\ll a_{k\uparrow}, a^+_{k\uparrow} \gg = 1 - \Delta \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg \qquad (3.1.12) \end{aligned}$$

where Δ is the energy gap

Let evaluate equation of motion for $\ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg$

$$\begin{aligned}\omega \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg= \quad & \delta_{kk'} + \ll [a^+_{-k\downarrow}, H_{BCS}], a^+_{k\uparrow} \gg \\ & = 0 + \ll [a^+_{-k\downarrow}, \sum_{p,p'} \epsilon_p a^+_{p,\sigma} a_{p',\sigma} - \sum_{p,p'} V_{p,p'} a^+_{p\uparrow} a^+_{-p\downarrow} a_{p'} \downarrow a_{-p'\uparrow}], a^+_{k\uparrow} \gg . \end{aligned} \tag{3.1.13}$$

$$\begin{aligned} I_3 = \quad & [a^+_{-k\downarrow}, \varepsilon_p a^+_{p\sigma} a_{p'\sigma'}], \\ & = \sum_p \varepsilon_p a^+_{p\sigma} \{a^+_{-k\downarrow}; a_{p'\sigma'}\} - \\ & \sum_p \varepsilon_p \{a^+_{-k\downarrow}; a^+_{p\sigma}\} a_{p'\delta'}, \qquad (3.1.14) \\ & = \sum_p \varepsilon_p a^+_{p\sigma} \{a^+_{-k\downarrow}; a_{p'\sigma'}\}, \\ & = \sum_p \varepsilon_p a^+_{p\sigma} \delta_{-kp'} \delta_{\downarrow\sigma}, \\ & I_3 = -\varepsilon_k a^+_{-k\downarrow}. \qquad (3.1.15) \end{aligned}$$

$$I_4 = [a^+_{-k\downarrow}, -\sum_{p,p'} V_{p,p'} a^+_{p\uparrow} a^+_{-p\downarrow} a_{p'} \downarrow a_{-p'\uparrow}]. \tag{3.1.16}$$

This evaluated to give

$$I_4 = V_p a^+_{p\uparrow} a^+_{-p\downarrow} a_{k\uparrow}. \tag{3.1.17}$$

Now upon putting I_3 and I_4 into equation no (3.1.13),

$$\begin{aligned} \omega \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg= \quad & \ll I_3, I_4 a^+_{k\uparrow} \gg, \\ & = -\epsilon_p \ll a_{-k\downarrow}, a^+_{k\uparrow}, \gg - \ll V_p a^+_{p\uparrow} a^+_{-p\downarrow} a_{k\uparrow} a^+_{k\uparrow} \gg \\ & (\omega + \epsilon_k)\omega \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg = -V_p a^+_{p\uparrow} a^+_{-p\downarrow} \ll a_{k\uparrow}, a_{k\uparrow} \gg \\ & (\omega + \epsilon_k)\omega \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg = -\Delta \ll a_{k\uparrow}, a_{k\uparrow} \gg \\ & \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg = \frac{-\Delta \ll a_{k\uparrow}, a_{k\uparrow} \gg}{(\omega + \epsilon_k)}. \qquad (3.1.18) \end{aligned}$$

(3.1.19)

But from equation no (3.1.12)

$$(\omega - \varepsilon_k) \ll a_{k\uparrow}, a^+_{k\uparrow} \gg = \quad 1 - \Delta \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg, \tag{3.1.20}$$

$$(\omega + \epsilon_k)\omega \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg = -\Delta \frac{(1 - \Delta \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg)}{\omega - \epsilon_k}, \tag{3.1.21}$$

$$(\omega + \epsilon_k)(\omega - \epsilon_k) \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg = -\Delta + \Delta^2 \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg . \tag{3.1.22}$$

$$\ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg = \frac{-\Delta}{\omega^2 - \varepsilon_k^2 - \Delta^2}. \tag{3.1.23}$$

(3.1.24)

Now the superconducting order parameter Δ,can begiven by the relation

$$\Delta = \frac{V}{\beta} \sum_k \ll a^+_{-k\downarrow}, a^+_{k\uparrow} \gg \tag{3.1.25}$$

upon substitution form equation no (3.1.24) into (3.1.25)

$$\Delta = \frac{V}{\beta} \sum_k \ll \frac{-\Delta}{\omega^2 - \varepsilon_k^2 - \Delta^2} \gg, \tag{3.1.26}$$

(3.1.27)

$$\sum \longrightarrow \int_{\varepsilon F}^{\infty} N(0) d\varepsilon,$$

$$\beta = 2N(0)V \int_0^{\hbar\omega} \frac{1}{\omega^2 - \varepsilon_k^2 - \Delta^2} d\epsilon,$$

changing $\omega \to i\omega$ and using the Matsubara fruquency,

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

$$\frac{1}{2N(0)V} = \int_0^{\hbar\omega} \frac{1}{(2n+1)^2\pi^2 + E_k^2\beta^2 + \Delta^2}. \tag{3.1.28}$$

$$Where \tag{3.1.29}$$

$$E_k^2 = \epsilon^2 + \Delta^2. \tag{3.1.30}$$

Using relation

$$\tag{3.1.31}$$

$$\frac{1}{2x}\sinh(\frac{x}{2}) = \sum \frac{1}{(2n+1)^2\pi^2 + x^2}. \tag{3.1.32}$$

$$\frac{1}{2N(0)V} = \frac{\beta}{2E_k\beta}\int_0^{\hbar\omega} \frac{\sinh(\frac{E_k\beta}{2})dE_k}{E_k}$$

$$= \ln u \tan u|_0^{\hbar\omega} - \int_0^{\hbar\omega} \frac{\ln y}{\cosh^2 y} dy.$$

For low temperature

$$\tan(\frac{\hbar\omega}{2k_BT}) \longrightarrow 1. \tag{3.1.33}$$

$$\frac{1}{2N(0)V} = \ln u - \ln(\frac{\pi}{4})e^{-c},$$

$$= \ln 1.14(\frac{\hbar\omega}{k_BTc}),$$

$$k_B T_c = 1.14\hbar\omega exp(\frac{-1}{N(0)V}),$$

$$k_B T_c = 1.14\hbar\omega exp(\frac{-1}{N(0)V}). \tag{3.1.34}$$

$$\tag{3.1.35}$$

Which is known BCS experession for superconducting tranision temperature.

3.2 Isotopic effect

It is widely accepted that isotope effect on T_c provide a strong evidence of superconducting mechanism that electron-phonon interaction is responsible for superconductivity in the frame work of BCS theory. Liu et al reported that the effect of isotopic substitution on T_c and an antiferromagnetic transition temperature T_N in $SmFeAsO_{1-x}F_x$ by replacing ^{16}O with isotope ^{18}O and $Ba_{1-x}K_xFe_2As_2$ by replacing ^{56}Fe with ^{54}Fe although T_N and T_c and found that the effect of oxygen isotope is much smaller than that of iron isotopic, which suggests that the FeAs layer is a conducting layer responsible for superconductivity [34]. In general an iron isotope coefficient (α) has estimated to be about 0.4 being close to 0.5 for full isotope effect in frame work of the BCS theory.These results seem to suggest the electron-phonon interaction play important role in superconductivity of iron-pnictide superconducters. Since these results are crucial for understanding the mechanism of iron pnictide superconductivity . Further experiments showing the variation in T_c in several experimental runs are highly desired [35]. According to BCS theory

$$T_C \sim M^{-\frac{n_1}{2}}. \tag{3.2.1}$$

where M is atomic mass and n_1 given by relation

$$n_1 = \frac{\lambda_{ph}}{\lambda_{ph} + \lambda_d}. \tag{3.2.2}$$

where λ_{ph} is coupling constant for phonon and λ_d is pairing coupling constant which in volving distortion field (df) (the cause of Jahn-Teller effect). Using the suitable values of the parameters for the system (LaOFFeAs) we calculated the value of α and the value for $(\lambda_{ph} = 0, 3)$ and $(\lambda_d = 0.09)$ because this constant parameters gives the experimental value of T_c for the system (LaOFFeAs) which given by workers on this area as listed refrance no [7].

Hence

$$\alpha = \frac{n_1}{2}. \tag{3.2.3}$$

using the above model the isotopic effect is calculated as

$$n_1 = \frac{0.3}{0.3 + 0.09} = 0.769. \tag{3.2.4}$$

$$\alpha = \frac{0.769}{2} = 0.3845 \approx 0.4. \tag{3.2.5}$$

which is almost experimental value of isotopic constant (0.4-0.5) for pnictide copounds

3.3 Model Hamiltonian

The degeneracy or near degeneracy of 3dxz and 3dyz may be the source of lattice distortion via Jahn-Teller or pseudo Jahn-Teller effects .The systems under study do exhibit structural instabilities due to tetragonal to orthorhombic distortion. This situation can be described by a two-level configurational distortion at each distorted tetrahedron at which the Fe ion exists.

A two-level system can be described by a pseudo spin ($S = \frac{1}{2}$) formalism [24]. Because

for every two-level system all 2x2 matrices and spin-half Pauli matrices along with 2x2 unit matrix form a complete set in the space of hermitian 2x2 matrices.

The Hamiltonian of a system of conduction electrons (in a narrow band) interactin with phonons and a distortion field (described by the two-level system) can be written as

$$H = H_e + H_c + H_{ph} + H_{e-ph} + H_{df} + H_{e-df}. \tag{3.3.1}$$

where

$$H_e = \sum_{\mathbf{k},\sigma} E_k C_{k,\sigma^+} C_{k,\sigma}. \tag{3.3.2}$$

$(C^{+,}_{k\sigma} C_k)$ being the electron (creation, annihilation) operators for the state $|k, \sigma >$ K is the wave vector, and σ the spin index. E_k is the single-particle energy. H_c is the screened Coulomb interaction between conduction electrons; H_{ph} is the standard phonon Hamiltonian; and He-ph is the electron-phonon interaction. H_{df} is the Hamiltonian of the distortion field that, in the pseudospin formalism, can be expressed as

$$H_{df} = -E_{as} \sum_m Sm^Z - ^{\frac{1}{2}} \sum_{i,m} J_{im} S_i^x S_m^x. \tag{3.3.3}$$

where i and m are site indices ,$E_{as} = E_a - E_s > 0$, being the energy difference between the two levels at site m and i. J_{im} denotes the interaction energy between distortion at sites i and m

$$H_{e-df} = \sum_{k-k'=q} V_d(k, k') C_{k'\sigma^+} C_{k\sigma} S_q^x. \tag{3.3.4}$$

which expresses the scattering of a conduction electron leading to a change in state of the

distortion field. The pairing coupling constant λ_d involving the distortion field (df) mode can be calculated by using the method described by Vujicic et al [38]. This yields

$$\lambda_d = \frac{N(0) < I_d^2 > E_{as} < S^Z >}{\omega_d^2}. \tag{3.3.5}$$

where ω_d is the average frequency of the distortion-field mode.

The phonon-mediated coupling constant is given by

$$\lambda_{ph} = N(0) < I_{ph}^2 >< \frac{1}{M\omega_{ph}^2} > . \tag{3.3.6}$$

where $< I_d^2 >$ and $< I_{ph}^2 >$ are the matrix elements of the corresponding interactions, N(o) is the density of electronic states at the Fermi level, ω_{ph} is the phonon frequency and M is the mass involved. We have also taken into account the role of phonons in the pairing process, though some workers have shown that the phonon contribution is too small [39]. The vertex function here is a sum of phononic and df modes [38].

3.4 Superconducting transition temperature (T_c)

In this section we try to calculate superconducting transition temperature (T_c) for (LaOFeFAs) using the siutable values of parameters with taking account of distortin mode between two levels (Jahn-Teller interaction). The expression for the critical temperature for the combined mechanism is given by;

$$T_c = 1.13(\omega_p)^{r_p}(\omega_d)^{r_d} exp(\frac{-1}{\lambda_{ph} + \lambda_d})[40]. \tag{3.4.1}$$

where

$$r_p = \frac{\lambda_{ph}}{\lambda_{ph} + \lambda_d}. \tag{3.4.2}$$

$$r_d = \frac{\lambda_d}{\lambda_{ph} + \lambda_d}. \tag{3.4.3}$$

Here we use the values of parameters to make numerical calculation and to compare those results with experimental value of superconducting transition temperature (Tc) for crosponding nictide superconducters. (We use the values of constant parameters($\lambda_{ph} = 0.2$), ($\lambda_d = 0.8$), (ω_{ph}=315.7K) as listed refrance no[40]. The value of ω_d depends on the separation of the two levels in question. As the unit cell contracts on applying pressure or by replacing La with Sm, Ce, Pd, Nd ions, which have smaller ionic radii ω_d will increase. The computed critical temperature values (for increasing values of ω_d) have been computed it by using these values of the parameters involved, by taking different values of distortion ferequence (ω_d) we will arive the effect of Jahn Teller interaction to superconducting transition temperatuure (T_c). For ($\omega_d = 40$), r_p= $\frac{0.2}{0.2+0.8} = 0.2$

T_c=1.13X$(315.7)^{0.2}(40)^{0.8}\exp(\frac{-1}{0.8+0.2}) \approx 26K$.

For (ω_d=50,)

T_c= 1.13 $(315.7\text{K})^{0.2}\times$ $(50)^{0.8}\exp(\frac{-1}{0.8+0.2})\approx$30K.

For(ω_d=75)

T_c=$1.13(315.7\text{K})^{0.2}(75)^{0.8}\exp(\frac{-1}{0.2+02})\approx$42K.

For($\omega_d = 100$)

T_c=$1.13(315.7\text{K})^{0.2}(100)^{0.8}\exp(\frac{-1}{0.2+02})\approx$53K.

For($\omega_d = 100$)

T_c=$1.13(315.7\text{K})^{0.2}(125)^{0.8}\exp(\frac{-1}{0.2+02})\approx$63K.

but this T_c value (63) is not yet discovered for iron pnictide superconducters until now but it may for future possibility to have this value for iron pnictide superconductors by any means of increasing by application pressure or replacing other elements [42].

distortion frequency(ω_d)	40	50	75	100	125
superconducting Tc in (K)	26	30	42	53	63

Table1 The calculated values of T_c for different distortion frequency(ω_d)

3.5 Energy gap

In 2008 the Hosono group discovered high temperature superconductivityin oxipnictide. The number, symmetry and amplitude of the gaps in the Fe-As superconductors are still open issues, as well as the origin of the electron pairing The experimental, the nature of the superconducting energy gap observed is very different from author to author and from and from sample to sample , ranging from one gap [41], two gaps and from isotropic gap or anisotropic full gaps to line node[42].

The ratio calculated for pnictide superconductors is different from BCS value$\frac{2\triangle}{K_B T_c}$ 3.52 [13,41].

In our case we considerethe energy gap is mediated due to phonon and distortion modes. According to referance no [12,40] The superconducting energygap (at T=0) is given by;

$$\triangle(0) = \lambda_{ph} \int_0^{\omega_{ph}} \frac{d\varepsilon \triangle_{ph}(0)}{[\varepsilon^2 + \Delta_{ph}^2(0)]^{\frac{1}{2}}} + \lambda_d \int_0^{\omega_d} \frac{d\varepsilon \triangle_d(0)}{[\varepsilon^2 + \Delta_d^2(0)]^{\frac{1}{2}}}. \tag{3.5.1}$$

where $\Delta_{ph}(0)$ and $\Delta_d(0)$ denote the energy gaps for the pure-phonon and distortion-mode parts.

Now let reduce above equation,

$$I_1 = \lambda_{ph} \int_0^{\omega_{ph}} \frac{d\varepsilon \triangle_{ph}(0)}{[\varepsilon^2 + \Delta_{ph}^2(0)]^{\frac{1}{2}}} and I_2 = \lambda_d \int_0^{\omega_d} \frac{d\varepsilon \triangle_d(0)}{[\varepsilon^2 + \Delta_d^2(0)]^{\frac{1}{2}}}. \tag{3.5.2}$$

using the integral

$$\int \frac{ydx}{\sqrt{x^2 + y^2}} = y \sinh^{-1}(\frac{x}{y}). \tag{3.5.3}$$

$$
\begin{aligned}
I_1 = \quad & \lambda_{ph}\int_0^{\omega_{ph}} \frac{d\varepsilon \triangle_{ph}(0)}{[\varepsilon^2+\Delta_{ph}^2(0)]^{\frac{1}{2}}}, \\
& = \lambda_{ph}\Delta_{ph}(0)\sinh^{-1}(\frac{\varepsilon}{\Delta_{ph}(0)}), \\
& = \Delta_{ph}(0)\lambda_{ph}Ln(\frac{\omega_{ph}}{\Delta_{ph}(0)}+\sqrt{(\frac{\omega_{ph}}{\Delta_{ph}(0)})^2+1}), \\
& = \Delta_{ph}(0)Ln(\frac{\omega_{ph}}{\Delta_{ph}(0)}+\sqrt{\frac{\omega_{ph}^2+\Delta_{ph}(0)^2}{\Delta_{ph}(0)^2}})^{\lambda_{ph}} \\
& = \Delta_{ph}(0)Ln(\frac{\omega_{ph}+\sqrt{\omega_{ph}^2+\Delta_{ph}^2}}{\Delta_{ph}(0)})^{\lambda_{ph}}, \\
& I_1 = \Delta_{ph}(0)Ln(\frac{\omega_{ph}+(\omega_{ph}^2+\Delta_{ph}(0)^2)^{\frac{1}{2}}}{\triangle_{ph}(0)})^{\lambda_{ph}}. \qquad (3.5.4)
\end{aligned}
$$

$$
\begin{aligned}
I_2 = \quad & \lambda_d\int_0^{\omega_d} \frac{d\varepsilon \triangle_d(0)}{[\varepsilon^2+\Delta_d^2(0)]^{\frac{1}{2}}}, = \lambda_d\Delta_d(0)\sinh^{-1}(\frac{\varepsilon}{\Delta_{ph}(0)}), \\
& = \lambda_d\Delta_d(0)Ln(\frac{\omega_d}{\Delta_d(0)}+\sqrt{(\frac{\omega_d}{\Delta_d(0)})^2+1}), \\
& = \Delta_d(0)Ln(\frac{\omega_d}{\Delta_d(0)}+\sqrt{\frac{\omega_d^2+\Delta_d(0)^2}{\Delta_d(0)^2}})^{\lambda_d}, \\
& = \Delta_d(0)Ln(\frac{\omega_d+\sqrt{\omega_d^2+\Delta_d^2}}{\Delta_d(0)})^{\lambda_d} \\
& I_2 = \Delta_d(0)Ln(\frac{\omega_d+(\omega_d^2+\Delta_d(0)^2)^{\frac{1}{2}}}{\triangle_d(0)})^{\lambda_d}. \qquad (3.5.5)
\end{aligned}
$$

(3.5.6)

$$
\Delta(0) = I_1+I_2 = \Delta_{ph}(0)Ln(\frac{\omega_{ph}+(\omega_{ph}^2+\Delta_{ph}(0)^2)^{\frac{1}{2}}}{\triangle_{ph}(0)})^{\lambda_{ph}}+\Delta_d(0)Ln(\frac{\omega_d+(\omega_d^2+\Delta_d(0)^2)^{\frac{1}{2}}}{\triangle_d(0)})^{\lambda_d}. \qquad (3.5.7)
$$

Here we try to made numerical calculation for energy gap at zero temperature using for different values of distortion frequency,taking the values of parameters listed in refrance no [40], ($\lambda_{ph} = 0.2$),($\omega_{ph} = 315.7K$) and $\lambda_d = 0.2$) and using equation no (3.5.7) The

calculated values are listed from the folling table

pnictide copounds	ω_d	T_c	$\Delta(_0)$in mev	$\frac{2\Delta(0)}{K_B T_c}$ in mev
LaOFFeAs	40	26	4.98	4.42
NdOFFeAs	50	30	5.48	4.23
CeOFFeAs	75	42	6.91	3.82
SmOFFeAS	100	53	8.13	3.78
?	125	63	10.70	3.93

Table2 The calculated values of T_c ,energy gap $\Delta(0)$ reduced energy gap and $\frac{2\Delta(0)}{K_B T_c}$ for different distortion frequency (ω_d)

Chapter 4

RESULT AND DISCUSSION

In previous section of chapter two we have studied the superconducting mechanism and the effect of structural distortion(Jahn-Teller effect)in this newly discovered iron pnictide compound(LaOFeAs). In chapter three, we try to calculated the values of the superconducting parameters by using right formula from recent journals listed in reference no [7,40]. Those parameters are;Isotopic coefficient (α) superconducting energy gap at zero temperature $\Delta(0)$ and reduced energy gap. Our calculated result clearly shows distortion (Jahn-Teller interaction) can have significant effect on superconducting parameters. The calculated T_c values for appropriate values of coupling constant for distortion mode (λ_d) and coupling constant of phonon (λ_{ph}) are found reference no [7,40]. It will be possible to produce experimental observed values of (Tc) and isotopic coefficient α and reduced gap. The exact calculation of superconducting parameters is better to starting from model Hamiltonian and it hasn't been attempted in the present because of the system is recently discovered and the problem of Jahn-Teller interaction is complicated to accomplish on short time. So evaluation of parameters are made from starting right formula listed

in reference no [40].The calculated values,rough estimates for(T_c ,α) and reduced gap ($\frac{2\Delta(0)}{K_BT}$) of different pnictide compounds are made for appropriate values of parameters seem to be reasonable agreement to the experimental values see table 1.The values of α that we get for pnictide compound is almost close to experimental value listed in reference no [35]. While our calculated values ($\frac{2\Delta(0)}{K_BT}$) which is substantially larger than the BCS value (3.52) as shown (table 2) indicates that strong coupling effects are important and the mechanism of superconducting is different. When distortion frequency (ω_d) increases the Tc values enhanced this reveals as distortion has significant effec .

Chapter 5

CONCLUSION

The superconductivity in newly discovered iron pnictide compound ($LaO_{1-x}F_xFeAs$) is being a big issue in condensed matter. This is because of the system contains ferromagnetic element iron (Fe).In this recently discovered pnictide compounds superconductivity is induced by substitution of suitable amount of F on O sites. the parent compound is unstable in its ground state. The instability is caused due to presence of degenerate Fe 3d orbitals. As result of interaction of degenerate electronic state the system is faced by Jahn-Teller effect. It is concluded that superconducting parameters;energy gap (Δ) no of pariticles inside Fermi surface(N(0)),coefficient of isotopic constant (α) are affected due to Jahn-Teller distortion,consequently superconducting transition temperature (Tc) is affected due to Jahn-Teller effect. The calculated parameters; coefficient of Isotopic constant (α) superconducting transition temperature(Tc) are almost exactly coincide with experimental values. The value of reduced gap ($\frac{2\Delta(0)}{K_BT}$) calculated is substantially larger than the BCS values(3.52) which reveals the strong coupling effect are important and the mechanism of superconducting in this system ($LaO_{1-x}F_xFeAs$)is different from BCS.

While distortion frequency increases Tc is enhanced. The enhancement of Tc can be made by increasing F doping or Pressure which enhance fluctuation in Fe 3d orbitals inside Fermi surface.

Finally as mentioned by different workers in this area ,the superconducting parameters are different from sample to sample as well as author to author. Also experimental values and calculated values are different.This reveals much work is reaming on this recently discovered pnictide compounds.

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Declaration

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

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Signature