STUDY OF COEXISTENCE OF THE SPIN-DENSITY WAVE AND SUPERCONDUCTIVITY IN FERROPNICTIDE($Ba_{1-x}K_xFe_2As_2$)

By

Sewnet Demelash

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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 "**COEXISTENCE OF SPIN DENSITY WAVE AND SUPERCONDUCTIVITY IN FERROPNICTIDE**($Ba_{1-x}K_xFe_2As_2$)" by **Sewnet Demelash** in partial fulfillment of the requirements for the degree of **Master of Science in Physics**.

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Approved by the examination commitee

Advisor: _____
ProfP.Singh

Examiners: _____
Prof.V.N.Mal'nev

_____
Prof.Javed Mazher

ADDIS ABABA UNIVERSITY

Date: **JUNE 2011**

Author: **Sewnet Demelash**

Title:

Department: **Physics**

Degree: **M.Sc.** Convocation: **JUNE** Year: **2011**

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Abstract

In this paper we study the relation ship between spin density wave(SDW) and superconducting order parameters in ferropnictides , the superconducting transition temperature and SDW transition temperatures.We use the Model Hamiltonian which is written in quantized form using annihilation and creation operators.We also study the coexistence of SDW and SC for $(Ba, K)Fe_2As_2$ system, the SDW-and superconductivity in an extended range of composition. The ternary iron arsenide $BaFe_2As_2$ becomes superconducting by hole doping which was achieved by partial substitution of the barrium site with potassium.We also investigate the effect of spin density wave on superconductivity, the coexistence of SDW and superconductivity for $(Ba_{1-x}K_xFe_2As_2)$ using phase diagram and the effect of doping on the transition temperature.

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Chapter 1

Introduction

1.1 The discovery of superconductivity

One of the many fascinating manifestations of strong correlations in materials is the presence of acondensate superconducting (SC) state in which all the electrons collapse into a unique electronic state for which the electrical current feels no resistance. Superconductivity was found in elemental materials such as mercury lead and tin a long time ago. In 1911 the Dutch physicist H. Kamerlingh-Onnes discovered a new fascinating natural phenomena often called superconductivity [1]. He wanted to measure the electrical resistance of different electrical materials.In a great astonishement he observed that the electrical resistance of mercury at temperature below 4.2 k was zero as shown in fig 1.1 . This temperature at which the jump of the electrical resistance is observed is called the critical temperature T_c.

The progress of superconductivity studies was very slow because one had to cool metals down to very low temperature and this task was not so simple these studies has to be carried out with liquid helium getting to few kelvin degrees. But the liquification of helium was itself another both interesting and difficult problem .It was twenty two years after Onnes discovery that the second fundamental properties of superconductors was revealed

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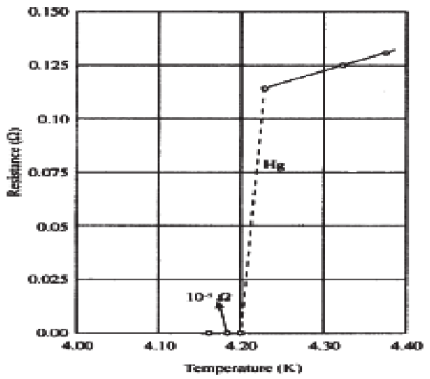

Figure 1.1: Electrical resistance of Hg at low temperature (Onnes 1911) which showed a transition temperature at 4.2 k.

1.2 Meissner effect

The Meissner effect is the expulsion of a magnetic field from a superconductor during its transition to the superconducting state.Walther Meissner and Robert Ochsenfeld discovered the phenomenon in 1933 by measuring the magnetic field distribution outside superconducting tin and lead samples.

The samples, in the presence of an applied magnetic field, were cooled below what is called their superconducting transition temperature.Below the transition temperature the samples cancelled nearly all magnetic fields inside.They detected this effect only indirectly; because the magnetic flux is conserved by a superconductor, when the interior field decreased the exterior field increased.The experiment demonstrated for the first time that superconductors were more than just perfect conductors and provided a uniquely defining property of the superconducting state.W.Meissner and R.Ochsenfeld[2] observed that superconducting sample was able to expel a constant but not very strong magnetic field out of it as shown in fig 1.2(a,b) and now we refer to this effect as the Meissner efffect.All materials in the superconducting state are strongly diamagnetic . The Meissner effect is really important, and it proves that the superconducting state is a reversible equilibrium state, a stable thermodynamic one, while for a simple perfect conductor the magnetic field history is important.The reversibility of the expulsion of a magnetic field

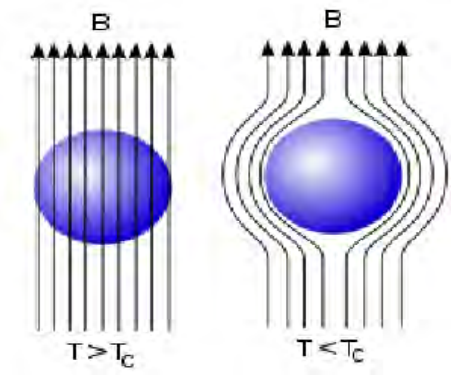

Figure 1.2: (a,b) Diagram of the Meissner effect. Magnetic field lines, represented as arrows, are excluded from a superconductor when it is below its critical temperature

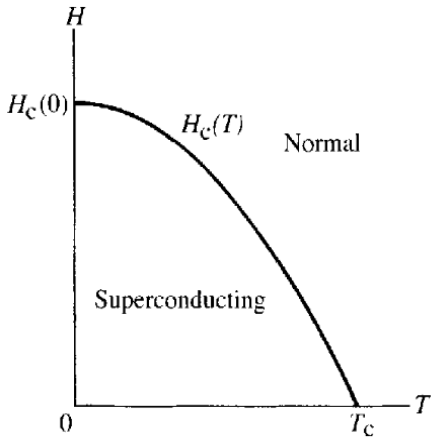

Figure 1.3: Phase diagram of a transition from the normal (N) to the superconductor (S) state.

from a superconductor implies that the transition between normal and superconducting state is reversible in temperature T and magnetic field H; thus there are two phases separated by a critical curve $H = H_c(T)$ as shown in Fig:1.3. Here we are referring to so called Type I superconductors, defined more precisely below.The critical field H_c can be related to the free energy difference between the normal and the superconducting state. To see this we have to define the thermodynamic potential energy density of both normal and superconducting state in presence of a magnetic field.Imposing their equality at the transition line we can obtain the expression that defines H_c.The thermodynamic potential

energy in a magnetic field is the Gibbs free energy, given by:

$$F(H,T) = F(T) - \frac{1}{4\pi}\int_0^H B(H')dH' \tag{1.2.1}$$

where F (T) is the Helmholtz free energy.In a superconductor, negleticing surface effects, B = 0, then:

$$F(H,T) = F_s(T) \tag{1.2.2}$$

while neglecting the much smaller response of the normal state, we can have B = H, then:

$$F_s(H,T) = F_n(T) - \frac{H^2}{8\pi} \tag{1.2.3}$$

Along the transition line $H = H_c(T)$ the two thermodynamic potentials are equal,so we obtain:

$$F_n(T) - F_s(T) = \frac{H_c^2}{8\pi} \tag{1.2.4}$$

This expression defines the thermodynamic critical field $H_c(T)$ as a function of the difference of free energy density between the normal and the superconducting phases.

1.2.1 Magnetic Levitation

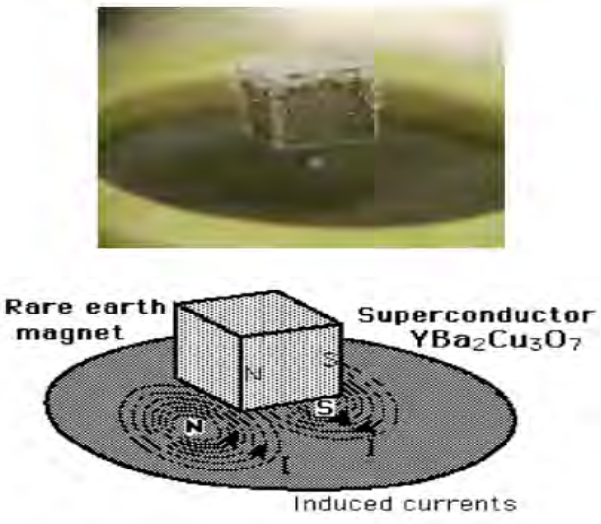

Figure 1.4: Meissner effect in superconductors like this black yitrium based superconductors

Magnetic fields are actively excluded from superconductors (Meissner effect).If a small magnet is brought near a superconductor,it will be repelled because induced supercurrents will produce mirror images of each pole.If a small permanent magnet is placed above a superconductor,it can be levitated by this repulsive force.The black ceramic material in the illustrations is a sample of the yttrium based superconductor. By tapping with a sharp instrument,the suspended magnet can be caused to oscillate or rotate.This motion is found to be damped, and will come to rest in a few seconds.[3]

1.3 London equation

In 1935 F.London and H.London show that the Meissner effect was a consequence of the minimization of the electromagnetic free energy carried by superconducting current[4]. They gave the first theoretical description of the behavior of a superconductor in a magnetic field. In an approximate way we can write down the following free energy for a superconductor into a magnetic field:

$$F = \int F_s(0) d^3r + E_{kin} + E_{mag} \tag{1.3.1}$$

where $F_s(0)$ is the free energy density of the condensed state, E_{kin} is the kinetic energy related to the current j_s , and E_{mag} is the magnetic energy due to the field H. But we have:

$$E_o = \int F_s(0) d^3r \tag{1.3.2}$$

$$E_{kin} = \int \frac{1}{2} m v^2 n_s d^3r \tag{1.3.3}$$

$$E_{mag} = \int \frac{H^2(\overrightarrow{r})}{8\pi} d^3r \tag{1.3.4}$$

where n_s is the superconducting electron density, and eq: (1.3.3) is valid only if the velocity (and thus the current j_s) is a spatially slow function. Now we have to remember the definition of the current and the Maxwell equation relating the magnetic field with

the current:

$$\overrightarrow{j_s} = ne\overrightarrow{v}(\overrightarrow{r}) \tag{1.3.5}$$

$$\overrightarrow{\nabla} \times H = \frac{4\pi j_s}{c} \tag{1.3.6}$$

where e is the electron charge; thus we can write the kinetic energy as:

$$E_{kin} = \int \frac{m j_s^2 n_s}{2n_s^2 e^2} d^3r = \int \frac{mc^2(\nabla \times H)^2}{2n_s e^2 (4\pi)^2} d^3r \tag{1.3.7}$$

Now we can rewrite the free energy for the superconductor as:

$$F = E_o + \frac{1}{8\pi} \int \Big[H^2 + \lambda_L^2 (\nabla \times H)^2 \Big] d^3r \tag{1.3.8}$$

where

$$\lambda_L = \sqrt{\frac{mc^2}{4\pi n_s e^2}}$$

this is the so called London length.

Now minimizing the free energy with respect to the variation of the field distributions $H(r)$ we can obtain the equilibrium state:

$$\begin{aligned} \delta F &= \frac{1}{4\pi} \int \Big[H.\delta H + \lambda_L^2 [\nabla \times H].[\nabla \times \delta H] \Big] d^3r \\ &= \frac{1}{4\pi} \int \Big[H + \lambda_L^2 [\nabla \times \nabla \times H \Big] d^3r = 0 \end{aligned} \tag{1.3.9}$$

this is the so called London equation

$$\Big[H + \lambda_L^2 \nabla \times \nabla \times H \Big] = 0 \tag{1.3.10}$$

1.4 The Landau-Ginzburg theory

In 1950 the phenomenological Ginzburg-Landau theory of superconductivity devised by Landau and Ginzburg[5].This theory which combined Landaus theory of second order phase transition with Schrodinger like wave equation had a great sucess in explaining macroscopic properties of superconductors.The phenomenological theory ,published by

Ginzburg and Landau in 1950, represents a remarkable acheivement of physical intuition. It is based on the more general theory of the second order phase transition developed by Landau himself; in a few words we can say that if there exists an order parameter Ψ which goes to zero at the transition temperature Tc ,the free energy may be expanded in power series of Ψ, and the coefficients of the expansion are regular functions of the temperature.Thus the free energy density is written as:

$$F = F_n + \alpha(T)|\Psi|^2 + \frac{\beta(T)|\Psi|^4}{2} + ..., \tag{1.4.1}$$

whereF_n is the free energy density of the normal state. The eq.(1.4.1) is limited to the case where the order parameter Ψ is a constant throughout the specimen. If Ψ has a spatial variation, then the spatial derivative of Ψ must be added to eq(1.4.1), and at the leading order we can write:

$$F = F_n + \alpha(T)|\Psi|^2 + \frac{\beta(T)|\Psi|^4}{2} + \gamma|\psi|^2 + ..., \tag{1.4.2}$$

Eq.(1.4.2) would not have been of a great help in the understanding of the properties of superconductors if Ginzburg and Landau had not proposed an extension to describe the superconductors in the presence of a magnetic field. With a great physical insight, they considered the order parameter ψ as a kind of electron wave function, and in order to ensure the gauge invariance they wrote the free energy density as:

$$F = F_n + \alpha(T)|\Psi|^2 + \frac{\beta(T)|\Psi|^4}{2} + \frac{1}{2m}|[-i\hbar\nabla - \frac{e^*\overrightarrow{A}}{c}]\psi|^2 + \frac{H^2}{8\pi}. \tag{1.4.3}$$

1.5 The BCS theory

In 1957 three American scientists J.Bardeen, L.Cooper and J.R Schrieffer [6] discovered the mechanism of superconductivity and now a days it is often called cooper pairing .It is a mile stone in the history not only in condensed matter but also in the entire physics.This theory explained superconducting current as superfluid of Cooper pairs,pairs of electrons

interacting through the exchange of phonons.The BCS theory the most significant theory that is used to describe the mechanism of superconductivity in low temperature superconductors (LTS) essentially pure metals and alloys such as Pb,Al, Ru,Nb_3Ge and their critical temperature is below 23k until the discovery of high temperature superconductors.Because of this reason all the mentioned substances are called conventionalsuperconductors.Following the microscopic quantum description of BCS theory low temperature heavy Fermions and low dimensional organic superconductors are discovered.

1.5.1 Successes of the BCS theory

BCS derived several important theoretical predictions that are independent of the details of the interaction,since the quantitative predictions mentioned below hold for any sufficiently weak attraction between the electrons and this last condition is fullfilled for many low temperature superconductors the so called weak-coupling case.These have been confirmed in numerous experiments:The electrons are bound into Cooper pairs,and these pairs are correlated due to the Pauli- exclusion principle for the electrons,from which they are constructed.Therefore,in order to break a pair,one has to change energies of all other pairs.This means there is an energy gap for single-particle excitation,unlike in the normal metal (where the state of an electron can be changed by adding an arbitrarily small amount of energy).This energy gap is highest at low temperatures but vanishes at the transition temperature when superconductivity ceases to exist.The BCS theory gives an expression that shows how the gap grows with the strength of the attractive interaction and the (normal phase) single particle density of states at the Fermi energy.Furthermore,it describes how the density of states is changed on entering the superconducting state, where there are no electronic states any more at the Fermi energy.The energy gap is most directly observed in tunneling experiments and in reflection of microwaves from superconductors.BCS theory predicts the dependence of the value of the energy gap E at temperature T on the critical temperatureT_c.The ratio between the value of the energy gap at zero

temperature and the value of the superconducting transition temperature (expressed in energy units) takes the universal value of 3.5, independent of material.Near the critical temperature the relation asymptotes to

$$E = 3.52 k_B T_c \sqrt{1 - (\frac{T}{T_c})} \tag{1.5.1}$$

Due to the energy gap, the specific heat of the superconductor is suppressed strongly (exponentially) at low temperatures,there being no thermal excitations left.However,before reaching the transition temperature,the specific heat of the superconductor becomes even higher than that of the normal conductor(measured immediately above the transition) and the ratio of these two values is found to be universally given by 2.5. It also describes the variation of the critical magnetic field (above which the superconductor can no longer expel the field but becomes normal conducting) with temperature. BCS theory relates the value of the critical field at zero temperature to the value of the transition temperature and the density of states at the Fermi energy. In its simplest form,BCS gives the superconducting transition temperature in terms of the electron-phonon coupling potential and the Debye cutoff energy:

$$k_B T_c = 1.14 \hbar \omega_D e^{(\frac{-1}{N(0)V})} \tag{1.5.2}$$

Here N(0) is the electronic density of states at the Fermi energy. The BCS theory reproduces the isotope effect, which is the experimental observation that for a given superconducting material,the critical temperature is inversely proportional to the mass of the isotope used in the material.

1.6 High T_c superconductors

According to BCS theory, superconductivity should not be possible above $\sim 30k$. Hence,all superconductors with higher critical temperatures are called high temperature superconductors (HTSC).

1.6.1 Cuprate superconductors

Over the years new superconducting materials were discovered and the superconducting temperature gradually increased.Until 1986 many scientist believed that superconductivity could not exist above 30k. It was this year that Bednorz and Muller discovered a lanthanum cuprate superconductor with a critical temperature of 35k[7].Not much later, lanthanum was replaced by yittrium, raising the critical temperature up to 92k.This was an important breakthrough because now much cheaper liquid nitrogen could be used as a coolant.Liquid nitrogen has a boiling point of 77k at atmospheric pressure.Since then many new cuprates have been discovered and the theory behind these superconducting materials is still a big challenge in condensed matter physics. Superconductivity was found in elemental materials such as lead and tin a long time ago, but it was not until 1986 with the discovery of high-temperature superconductivity in copper oxides that the dream of making these materials useful inspired and challenged many generations of physics. Cuprates are based on layers of copper and oxygen sandwiched between other elements such as La, Ba, Sr or other atoms which stabilize the crystal structure.Electrons or holes are doped in the copper-oxide layers. Cuprates superconductors crystallize in the perovskite structure, see Fig:1.5(b). In Fig:1.5(a) a qualitative phase diagram is shown for the cuprate superconductors. For the undoped parent compounds there is a transition at T_N from paramagnetic to the anti-ferromagnetic phase, no superconductivity is observed. When the doping level is increased, T_N is decreased, and around the point were the magnetic transition is almost completely suppressed the superconducting dome (SC) starts. For underdoped and optimal doped cuprates there is also a pseudogap. For higher doping levels the pseudogap disappears and the superconducting transition temperature decreases. The current recordT_c of 164k was achieved in the cuprate $HgBa_2Ca_2Cu_3O_{8+}(Hg1223)$ with an ambient T_c of 134k, under a pressure 30 GPa.[3]

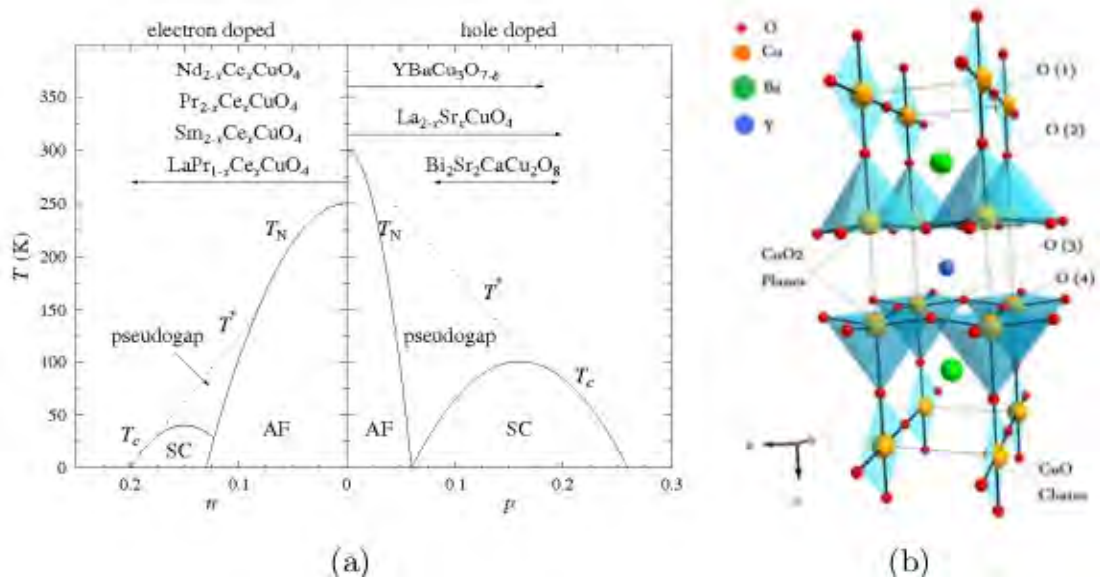

Figure 1.5: (a) Simplified doping dependent phase diagram of cuprate superconductors for both electron (n) and hole (p) doping. (b) Crystal structure of a YBCO cuprate superconductor.

1.7 Iron based superconductors

The first superconducting iron oxypnictide was discovered in 2006, based on phosphoruss uch as LaOFeP with 5k and LaONiP with 3k which has not attracted much attention. When phosphorus was substituted by arsenic there was drastic increase in critical temperature.The oxypnictide shows the layered structure like cuprates.They have common ZrCuSiAs type crystal structure belonging to the tetragonal P_4/nmm space group.Besides these quaternary REOFeAs (1111) oxypnictide superconductors several high T_c superconductors have been discovered also in other Fe based analogues compounds including ternary compound AFe_2As_2 (A is an alkali earth metal element such as Sr and Ba). By synthesis of$Ba_{1-x}K_xFe_2As_2$ superconductivity was observed with a critical temperature $T_c = 38K$.This compound is known as (122).(The numbers referring to the ratio of the elements in the compound in order of sequence.) A completely new class of high-temperature superconductors containing iron coordinated with pnictogen atoms (such as As or P), called iron pnictides, was discovered in 2008 [8] and their pairing symmetry is

still under investigation .It is not yet clear whether the mechanism for superconductivity in these iron-based superconductors is closely connected to that in cuprates or whether a new route to high-temperature superconductivity has been found.In this thesis, we will review the recent experimental developments in the study of the electronic properties of iron pnictides,highlighting the role of the Fermi surface topology.Since the discovery of cuprates in 1986 no other material has reached a superconducting transition as high as 55k.The discovery in early 2008 of the new class of high temperature superconductors has broken the monopoly of the cuprates in the physics of high temperature superconducting compounds.At present dozens of HTSC compounds are known to have of superconducting transitions T_c temperatures exceeding 24k. After more than 20 years the cuprates are the most extensively studied class of compounds in condensed matter physics.While superconductivity in conventional metals is well understood by the BCS theory,the mechanism that is responsible for the pairing of carriers in the cuprates is far from being clear.Besides cuprates there are some other superconductors in the HTSC group.The superconducting transition temperature vs year of discovery for LTS metals ,alloys compounds and HTSC compounds is shown in fig:1.6

On the other hand,the magnetic nature of the parent compound seems to favor a coupling mechanism based on nesting-related anti-ferromagnetic spin fluctuations [9].In this case an interband sign reversal of the order parameter between different sheets of the Fermi surface (symmetry) is predicted.The number, amplitude, and symmetry of the superconducting energy gaps are indeed fundamental physical quantities that any microscopic model of superconductivity has to account for.In recently discovered iron pnictide materials superconductivity(SC) and spin density wave (SDW) states are close neighbor[10].The interplay between these two orders has been the focus of numerious experiment and theoretical studies.Superconductivity and magnetic ordering are normally mutually exclusive states of electronic systems and first order transition between superconductivity and spin density wave orders has been reported in some pnictides. However,recent nuclear magnetic

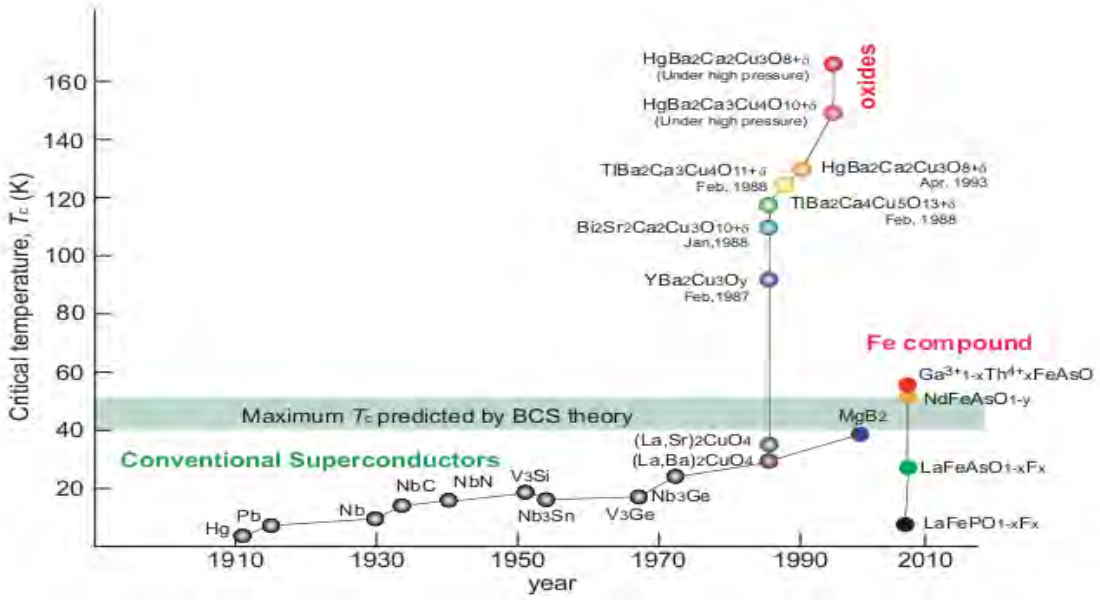

Figure 1.6: The superconducting transition temperature vs year of discovery for LTS metals ,alloys ,compounds and HTSC compounds

resonance(NMR)[11] and neutron scattering(NS)[12] experiment on $Ba(Fe_{1-x}Co_x)_2As_2$ indicates that SDW and SC phases coexist over some doping range.

1.7.1 Crystal structure and physical properties of pnictides

The crystal structures of the four families of iron pnictides are discussed briefly below:

1111 family

LaFeAsO and the 1111 family of iron pnictides crystallizes in the ZrCuSiAs- type structure, (space group P4/nmm). In this structure, two-dimensional layers of edge-sharing $FeAs_4/4$ tetrahedra alternate with sheets of edge- sharing $OLa_4/4$ tetrahedra as shown in Fig(a). Because of the differences between the ionic nature of the Ln-O (Lanthanum oxide) bonds and the more covalent Fe-As (iron arsenide) bonds, a distinctivetwo-dimensional structure forms, where ionic layers of lanthanum oxide $(LaO)^+$ alternate with metallic layers of iron arsenide $(FeAs)$.

122 family

The ternary iron arsenide $BaFe_2As_2$, with the tetragonal $ThCr_2Si_2$ -type structure

space group (space group I_4/nmm) contains practically identi- cal layers of edge-sharing $FeAs_4/4$ tetrahedra, but they are separated by barium atoms instead of LaO sheets. This structure is shown in Fig (b)

111 family

LiFeAs crystallizes into a Cu_2Sb-type tetragonal structure containing [FeAs] layer with an average iron valence Fe^{2+} like those for 1111 or 122 parent compounds. This structure is shown in Fig:(c)

11 family

The PbO-type FeSe crystal structure is shown in Fig:(d) Here some physical properties of iron pnictides:

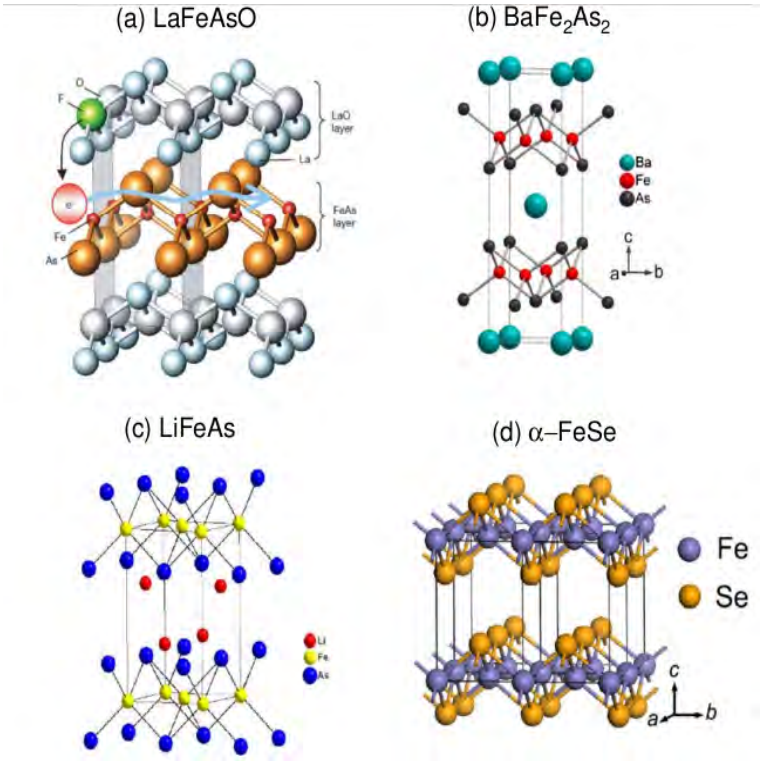

Figure 1.7: Schematic crystal structure of: (a) LaFeAsO, (b) $BaFe_2As_2$ (c) LiFeAs (d) FeSe

The transition temperature for different compounds of iron pnictides is also shown in the table 1.

The maximum transition temperature for 1111family is 56k and 38k for 122 family.This

discovery of iron based superconductors breaks the monopoly of cuprate compounds as shown in table 1.

Material(Iron compounds) doped 1111Family	Maximum Transition Temperature(Tc in K)	Material(Iron compounds) doped 122Family	Maximum Transition Temperature(Tc in K)	SCOP(Δ in mev)for 122 families
$SmFe_{1-x}Ni_xAsO$	10	$Sr(Fe_{1-x}Pd_x)_2As_2$	9	2.36
$LaFe_{1-x}Ir_xAsO$	12	$Sr(Fe_{1-x}Ni_x)_2As_2$	10	2.63
$LaFe_{1-x}Co_xAsO$	14	$Sr(Fe_{1-x}Ru_x)_2As_2$	13.5	3.56
$LaFeAsO_{1-x}F_x$	26	$Ca(Fe_{1-x}Co_x)_2As_2$	17	4.48
$CeFeAsO_{1-x}F_x$	41	$Ba(Fe_{1-x}Pd_x)_2As_2$	19	5.01
$DyFeAsO_{1-x}F_x$	45	$Ba(Fe_{1x}Ni_x)_2As_2$	20	5.27
$TbFeAsO_{1-x}F_x$	46	$Ba(Fe_{1-x}Ru_x)_2As_2$	21	5.54
$PrFeAsO_{1-y}$	48	$Sr(Fe_{1-x}Rh_x)_2As_2$	22	5.08
$GdFeAsO_{1-x}F_x$	50	$Sr(Fe_{1-x}Ir_x)_2As_2$	22	5.08
$PrFeAsO_{1-x}F_x$	52	$Ba(Fe_{1-x}Co_x)_2As_2$	22-24	5.08-6.33
$GdFeAsO_{1-x}F_x$	52	$Ba_{1-x}Rb_xFe_2As_2$	23	6.07
$TbFeAsO_{1-y}$	52	$Ba(Fe_{1-x}Rh_x)_2As_2$	24	6.33
$DyFeAsO_{1-y}$	52	$Ba(Fe_{1-x}Rh_x)_2As_2$	25	6.59
$GdFeAsO_{1-y}$	53	$Eu_{1-x}K_xFe_2As_2$	32	8.44
$NdFeAsO_{1-y}$	53	$Eu_{1-x}Na_xFe_2As_2$	35	9.23
$SmFeAsO_{1-x}F_x$	55	$K_{1-x}Sr_xFe_2As_2$	36	9.49
$SmFeAsO_{1-y}$	55	$Cs_{1-x}Sr_xFe_2As_2$	37	9.76
$Gd_{1-x}Th_xFeAsO$	56	$Ba_{1-x}K_xFe_2As_2$	38	10

Table 1.1: Summary of the maximum transition temperatures at ambient pressure for various Fe-based superconductors

Chapter 2

Review of Literature

2.1 Coexistence of superconductivity and Spin density wave in $Ba_{1-x}K_xFe_2As_2$

2.1.1 Superconductivity in hole doped $BaFe_2As_2$($Ba_{1-x}K_xFe_2As_2$)

Iron is one of the most abundant metal on the surface of the earth and has been known as a useful element since aptly named Iron age.However,it wasnot untill recently that when combined with element from the group five and group six of the periodic table (named respectively thepnictogen after the Greek verb for choking and chalcogen meaning ore formers) .Iron based metals were shown to readily harbour a new form of high temperature superconductivity.This general family of materials has quickly grown to be large in size with well over 50 different compounds identified that show a superconducting transition that occurs at temperature approaching 60k and includes different varieties of iron and nickel based systems.

In this thesis the properties of parent compound $BaFe_2As_2$ and doped $Ba_{1-x}K_xFe_2As_2$ are studied.The $BaFe_2As_2$ crystallizes in the tetragonal $ThCr_2Si_2$ -type structure with two formula units per unit cell space group I4/mmm and crystal parameters a=0.39435 nm and c=1.3118 nm. Like in oxypnictides the crystal structure is layered and formed by edge sharing $FeAs_4/4$ tetrahedrons with covalent bonding, interlaced by the layers of

Ba^{2+} sheetsperpendicular to [001] instead of (La-O) layers for LaOFeAs.The interlayer bonding is ionic,like oxypnictides. The quasi two dimensional characters of both compounds make them similar to the well studied class of superconducting copper oxides. The metal- metal bonding within the layers plays an important role in the properties of $ThCr_2Si_2$ type structure. Assuming the iron atoms are in the Fe^{2+} state ($3d^6$) the d shell is more than half filled and Fe-Fe anti bonding states should be at least partially occupied. The lowest lying bands are made by the overlap of the Fe-$3d_{x^2y^2}$ orbital. Hence, the undoubtedly present Fe-Fe bonds (Fe-Fe=0.2802 nm) in $BaFe_2As_2$ are slightly weakened, but more important less dispersed and mainly responsible for the magnetic properties. At 140 k $BaFe_2As_2$ undergoes a structural phase transition from tetragonal (I4/mmm) to orthorhombic (Fmmm) space group. It can be seen that for $BaFe_2As_2$ compound the Fe-As distance is smaller than LaOFeAs.So there is more considerable Fe-d-As-p hybridization, for $BaFe_2As_2$ system in comparison with $LaOFeAs$.It is stronger than the latter and as a result has a wider Fe-d bandwidth. The distance between the nearest Fe atoms within FeAs layers is also significantly smaller in AFe_2As_2 as compared with $LaOFeAs$ system. After the structural transition to the orthorhombic structure the Fe-Fe distances are separated into two types of band width out of four bonds, the two pairs of bonds have a width of 0.2802 nm and the other two pairs have the width of 0.2877 nm. The angles between the Fe-As-Fe are also different than the oxypnictide systems. Such a difference in the adjacent Fe ions should lead to changes in their electronic structure.As mentioned earlier similar to the oxypnictide systems the structural and magnetic transition also occurs in the AFe_2As_2.Superconductivity can be recovered by substituting the A ions by some impurity holes.The compound was doped by the chemical substitution of A^{2+} ions by potassium ions (K^+). While electrons are doped by the replacement of divalent iron atoms with trivalent cobalt (Co) or tetravalent nickel (Ni) ions T_c can be enhanced by applying pressure on doped or undoped compounds. The difference between the two systems regarding structural and magnetic transition are,in oxypnictide both the

structural and magnetic transition occurs at different temperature .The magnetic transition occurs 10 to 20 k lower than the structural transition. While in AFe_2As_2 compounds it is found coupled and for same transition temperature. [13].

The second class (AFe_2As_2 with A block as the charge reservoir and A may represent(Sr, Ba,Ca or in general alkali and alkaline earth metals) and A may be substituted doping one impurities .

2.1.2 Electronic and crystal structure of $Ba_{1-x}K_xFe_2As_2$

The properties of parent compound $BaFe_2As_2$ and doped $Ba_{1-x}K_xFe_2As_2$ are studied in detail in this thesis.The $BaFe_2As_2$ crystallizes in the tetragonal $ThCr_2Si_2$type structure with two formula units per unit cell space group I_4/mmm and crystal parameters a=0.39435 nm and c= 1.3118 nm.Like in oxypnictides the crystal structure is layered and formed by edge sharing $FeAs_4/4$tetrahedrons with covalent bonding, interlaced by the layers of Ba^{2+} sheets perpendicular to [001] instead of (La-O) layers for LaOFeAs.The interlayer bonding is ionic, like oxypnictides.The quasi two dimensional characters of both compounds make them similar to the well studied class of superconducting copper oxides.The metal- metal bonding within the layers plays an important role in the properties of $ThCr_2Si_2$- type structure. Assuming the iron atoms are in the Fe^{2+}state ($3d^6$) the d shell is more than half filled and Fe-Fe anti bonding states should be at least partially occupied.The lowest lying bands are made by the overlap of the Fe-$3d_{x^2-y^2}$ orbital. Hence, the undoubtedly present Fe-Fe bonds (Fe-Fe=0.2802 nm) in $BaFe_2As_2$ are slightly weakened, but more important less dispersed and mainly responsible for the magnetic properties.

The family of FeAs based superconductors has been extended to double layered ternary iron arsenide AFe_2As_2 (A= Sr, Ba, Ca, Eu) (A: Alkali metals and Alkali -earth metals), so-called 122 systems.The ternary iron Arsenide AFe_2As_2 with tetragonal $ThCr_2Si_2$ type structure was first suggested by Rotter ref [14] it contains, identical edge sharing $FeAs_4$ tetrahedra. The crystal structure is similar to that of layered REOFeAs, only the REO is

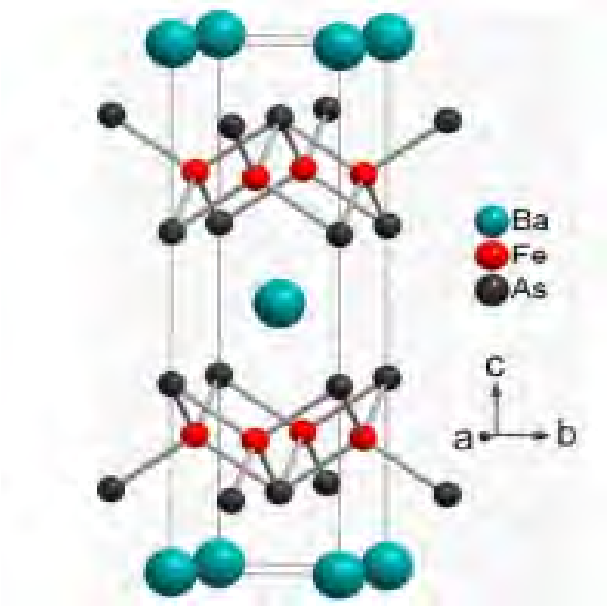

Figure 2.1: Shows the crystal structure of$BaFe_2As_2$ [14]

replaced by the Ba sheet in between FeAs layers.It does not contain oxygen which means that it not only breaks the monopoly of cuprates but also proved that the superconductivity of FeAs based superconductors are not associated with oxygen layers.The crystal structure of $BaFe_2As_2$ is shown in fig:2.1

[15] $BaFe_2As_2$ is a poor Pauli-paramagnetic metal that undergoes a structuraland magnetic phase transition at 140k, accompaniedby strong anomalies in the specific heat, electrical resistance and magnetic susceptibility.In the course of thisphase transition, the space group symmetry changes from tetragonal (I_4/mmm) to orthorhombic (F mmm).Based on these findings, we expected superconductivity in doped $BaFe_2As_2$.First attempts to realize electron doping by lanthanum substitution were unsuccessful,because the required doping level could not be achieved.Researchers then decided to try hole doping by substituting theBa^{2+} cations for K^+ with a similar ionic radius.

It can be seen that for $BaFe_2As_2$ compound the Fe-As distance is smaller than LaOFeAs. So there is more considerable Fe-d-As-p hybridization,for $BaFe_2As_2$ system in comparison with LaOFeAs.It is stronger than the latter and as a result has a wider Fe-d bandwidth.The distance between the nearest Fe atoms within FeAs layers is also

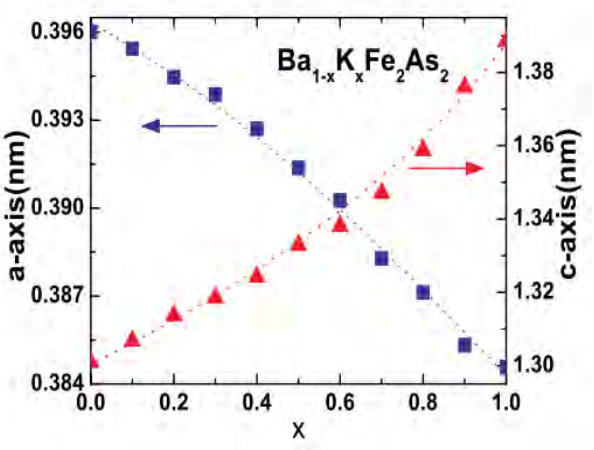

Figure 2.2: Dependence of the lattice parameter with composition(16)

significantly smaller in AFe_2As_2 as compared with $LaOFeAs$ system.After the structural transition to the orthorhombic structure the Fe-Fe distances are separated into two types of band width out of four bonds, the two pairs of bonds have a width of 0.2802 nm and the other two pairs have the width of 0.2877 nm.The angles between the Fe-As-Fe are also different than the oxypnictide systems.Such a difference in the adjacent Fe ions should lead to changes in their electronic structure. As mentioned earlier similar to the oxypnictide systems the structural and magnetic transition also occurs in the AFe_2As_2.Superconductivity can be recovered by substituting the A ions by some impurity holes.The compound was doped by the chemical substitution of A^{2+} ions by potassium ions (K^+). The difference between the $BaFe_2As_2$ and oxypnictides regarding structural and magnetic transition are, in oxypnictide both the structural and magnetic transition occurs at different temperature.The magnetic transition occurs 10 to 20k lower than the structural transition. While in AFe_2As_2 compounds it is found coupled and for same transition temperature. Thelattice parameter dependence on the composition of the sample at room temperaturefor $Ba_{1-x}K_xFe_2As_2$ is shown in fig:2.2. It is found that the changes are continuous and linear.The structural changes mainly affect the Fe-Fe bond length and the angle between the Fe and As.

The anomaly associated with the structural and magnetic transition is pronounced

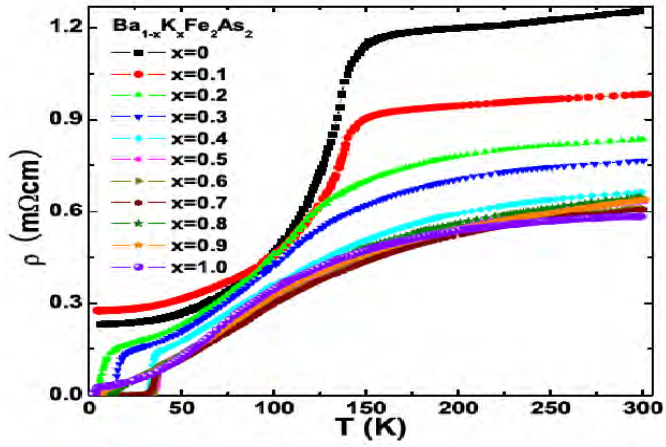

Figure 2.3: Temperature dependence of the resistivity

for x = 0 and x=0.1.The anomaly is rounded off for x = 0.2, which becomes a superconductor with the transition starting at 14k and the resistivity reaching zero at 3k as shown in fig:2.2. The T_C increases with further potassium doping and the superconducting transition becomes narrower until x = 0.5. Thereafter, T_C begins to decrease from the maximum $T_C \approx 37.5$k with the increasing potassium doping. At x = 1, T_C is 3.8 K forthe KFe_2As_2 sample,the same as reported by Sasmal et al. [17].

There is hope that doping of this and related materials could lead to an increase in transition temperature.

2.1.3 Magnetic Ordering in $Ba_{1-x}K_xFe_2As_2$

This was first observed in LaFeAsO where the magnetic structure was characterized by the ordering wavevector $(\frac{1}{2}\frac{1}{2}\frac{1}{2})_T = (10\frac{1}{2})_O$ (where the subscripts T and O refer to the tetragonal and orthorhombic structures, respectively) and the low temperature ordered magnetic moment was $0.36\mu_B$ [13].At this point, we note that the ordering wavevector in the orthorhombic cell i.e.$(10\frac{1}{2})_O$ differs from the wavevector listed in [20] as the later wavevector is relative to the unit cell of the magnetic structure where the unit cell is doubled along the c-axis. The observed wavevector is consistent with a magnetic unit cell ofsize$\sqrt{2}a \times \sqrt{2}a \times 2c$ relative to the tetragonal cell.This ordering is consistent with stripe

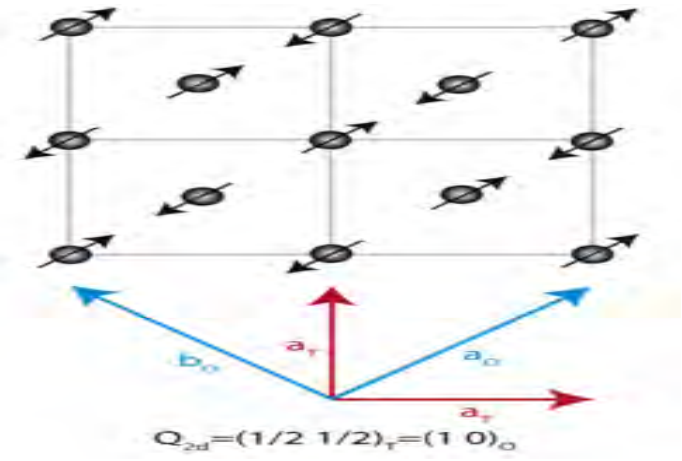

Figure 2.4: In-plane magnetic structure for 122 parent compounds the ordering wave vector in these compounds is$(\frac{1}{2}\frac{1}{2}L)_T$=$(10L)_O$,for 122 families , the stacking is antiferromagnetic along the c-axis resulting in odd integers L as the unit cell contains two FeAs layers.

like anti-ferromagnetic order with ferromagnetically coupled chains along the tetragonal (1 1 0) direction coupled antiferromagnetically along the in -plane perpendicular direction as shown in fig:2.4.The doubling of the unit cell along the c-axis indicates anti-ferromagnetic interactions between neighboring planes.The magnetic moment direction could not be uniquely determined in this measurement but the observed intensity is consistent with moments lying in the a-b plane.

Magnetic ordering(structure) of parent compounds $BaFe_2As_2$ can be determined using comprehensive neutron experiment and peculiar coexistence of superconductivity and spin density wave ordering in the underdoped region of $BaFe_2As_2$.Doped $BaFe_2As_2$ ($Ba_{1-x}K_xFe_2As_2$)have attracted tremendous amount of attention in the quest to understand the mechanism of high transition temperature superconductivity.Neutron scattering has been playing adecisive role in the understanding of structural and magnetic properties of Iron pnictides as demonstrated from the first observation of anti-ferromagnetic ordering of the Iron moment in LaFeAsO via neutron powder diffraction.Spin density wave ordering from itinerant Fe spins is believed to be responsible for anti-ferromagnetism.It has also been established that magnetic ordering in Iron pnictides is strongly coupled to

lattice instabilities.Superconductivity emerges up on electron or hole doping via chemical substitution.

Undoped compounds show some magnetic orders in both system but the starting point are very different ,a Mott insulator in the cuprates and antiferromagnetic (SDW) metal in the Fe compounds.This difference suggests that the electron interaction is strong in the cuprates whereas it is moderate or weak in the pnictides .The effect of doping looks very different,doping in to the Mott insulating cuprates causes reconstruction of states on a large energy scale while the doping in to Fe-pnictides seems to only shift the chemical potential with out appreciable change of band structure.

A different view point might emerge if one looked at the spin structure of undoped Fe-pnictides ordered ferromagnetically in one direction and antiferromagnetically in the other direction in the square Fe-plane,this looks like stripe spin order.The stripe order can be easily destroyed by doping, by introduction of foreign atoms and by applying pressure. Long range magnetic ordering shares similar pattern in all of Fe-As based superconducting systems as shown in the projection of the square lattice in fig :2.5.The iron sublattice undergoes magnetic ordering with an arrangement consisting of spins ferromagnetically along one chain of nearest neighbours with in iron lattice plane and anti-ferromagnetically arranged along the other directions.

2.2 Spin density wave in ferropnictide($Ba_{1-x}K_xFe_2As_2$)

Spin density wave (SDW) is a kind of anti-ferromagnetic state with electron spin density forming a static wave.The density varies perpendicularly as afunction of position with no net magnetization in the entire volume.The spin density wave(SDW) transition occurs when the spatial spin density modulation is due to delocalization or initinerant electrons rather than localized one. Usually in the normal state the density$\rho\uparrow(r)$ of electron spins polarized upward with respect to any quantization axis is completely cancelled by$\rho\downarrow(r)$ of

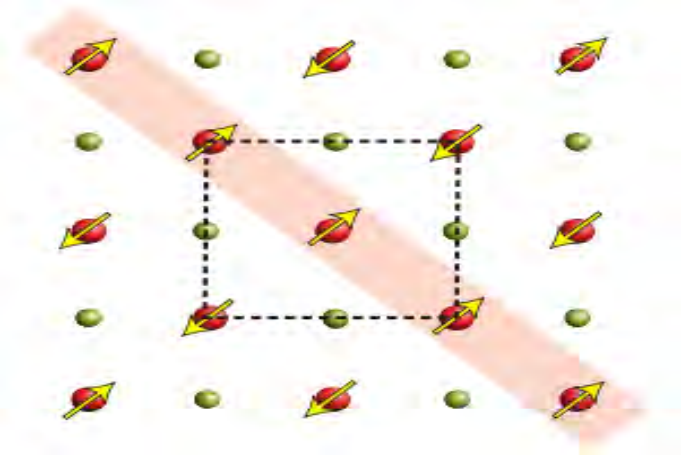

Figure 2.5: The active planar iron layer common to all superconducting compounds with iron ions

down ward polarized spins . In the spin density wave state (SDW) ,however,the differenc $\sigma(r) = \rho \uparrow (r) - \rho \downarrow (r)$ is finite and modulate in space as a function of the position vector in the spin density wave state. Such tendency offorming SDW ground state takes place when apossesses nested pieces of Fermi- surface together with intermediate coloumb correlation structure, of alternating layers of Fe-As and Re-O layers where FeAs layers are thought to be responsible for superconductivity.The parent compound or undoped compound of these systems is not superconducting itself and exhibits both a structural and magnetic phase transition.This structural phase transition changes the crystal symmetry from tetragonal (space group P4/nmm) to orthorhombic (space group Cmma) and leads to an anti-ferromagnetical order with a spin structure which is shown in figure:2.6

The superconductivity emerging from these SDW compounds is theoretically proposed to be unconventional and mediated by AFM spin fluctuations.Such an SC state has an extended s-wave pairing with a sign reversal of the order parameter between different Fermi surface sheets, as the magnetic fluctuations,while too broad to induce a magnetic instability, are instrumental in stabilizing superconductivity.

There is lot of experimental and theoretical work giving evidence that the anomaly caused by a SDW. As a function of temperature the resistivity of the undoped parent

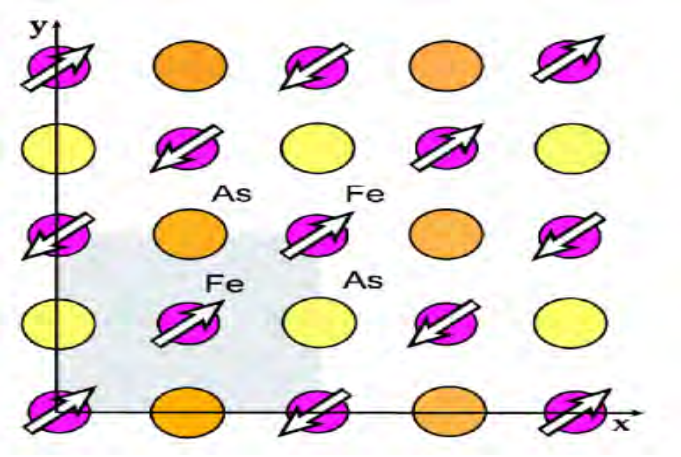

Figure 2.6: The spin-density-wave (SDW) order as observed by the neutron diffraction. The Fe magnetic moments along the (1, 1) direction are aligned, while the two nearest neighboring Fe are antiferromagnetically aligned

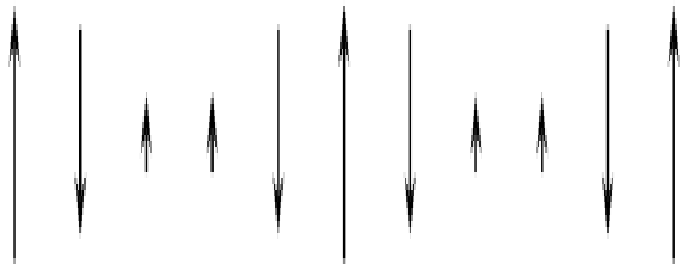

Figure 2.7: SDW

compound, which is not an insulator like the cuprates shows a drop around 150K, which shows the structural transition from tetragonal at high temperature to orthorhombic at low temperature.Furthermore the neutron diffraction studies showed that around 130K while still in monoclinic phase the compound develops a spin density wave. 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 origin of the SDW is commonly attributed to the nesting properties of the Fermi surface, which determines the wave vector q of the SDW as shown in fig:2.8. The first neutron scattering experiments on Chromium by Neel (1936) [18] found that the magnetic ground state is described through antiferromagnetic (AFM) order. Upon a deeper view though, Shull and Wilkinson (1953) [19] detected that the ground state is rather a spin density wave (SDW), meaning that the moment is varied sinusoidally.This is a generalisation of the AFM state, which can be interpreted as a special case of a commensurate SDW state with wave vector of $q = \frac{a_z}{2}$,$a_z = \frac{4\pi}{a} e_z$,being the unit vector in z direction in the reciprocal space.

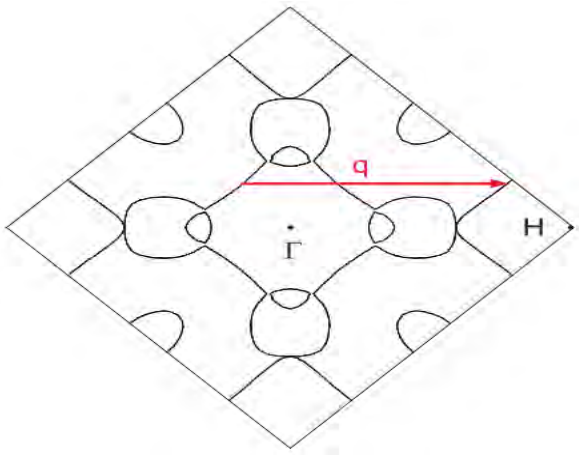

Figure 2.8: Nesting properties of Fermi-surface which shows an electron surface centred at Γ and a hole surface centred at$H$

2.3 Phase diagram for coexistence of superconductivity and spin density wave in $Ba_{1-x}K_xFe_2As_2$

The basic behavior of the superconducting materials canbe described by considering the phase diagrams for$Ba_{1-x}K_xFe_2As_2$ (hole doping between the FeAs planes) and materials share the same $BaFe_2As_2$ parent compound.

As mentioned previously,the AFe_2As_2 in the case of , Ba-122 exhibits both a structural phase transition (in this case from the room temperature tetragonal I_4/mmm space grouped to the low temperature orthorhombic Fmmm space group [21]) and the magnetic transition to a long range ordered, SDW state.However,unlike the 1111 materials, both the structural and magnetic phase transitions occur at the same temperature in the Ba-122 parent compound [22]. Doping with K [21] causes a suppression of the structural and SDW transitions as in the 1111 materials.In doping potassium ,superconductivity emerges as the SDW order is suppressed. For K doping,the superconducting region starts for x= 0.1 and the maximum T_C of 38 K is for x= 0.4 Interestingly, for K doping, there is a region of the phase diagram where the SDW state and structural transition coexist with superconductivity. Coexistence of superconductivity and magnetism has been a recurring theme in the study of superconductingmaterials [23].

For the doped 122 materials, the question of whether the SDW and superconducting states are microscopically coexisting or phase separated has received considerable attention experimentally.For hole doping with K, 75 As NMR [24], SR [25] and magnetic force microscopy [26] consistently indicate distinct regions which are magnetically ordered and nonmagnetic regions as expected for microscopic phase separation. Furthermore, analysis of microstrain measured with x-ray and neutron diffraction was interpreted as being consistent with electronic phase separation [27].Although most measurements on the K doped samples are consistent with a phase separation scenario,57Fe-M ssbauer measurements indicate a sample which is completely magnetically ordered as expected with microscopic coexistence of the SDW and superconducting states [28].

For the case of Co doping, both 75As NMR [29] and SR measurements [30] indicate that all the Fe sites participatein the magnetic order as would be expected for coexistenceof superconductivity and SDW order.One 75 As NMR study directly compared the cases of K and Co doping and concluded phase coexistence for Co doped samples and separation for the case of K doping [31].Finally,neutron diffraction measurements on Co doped

samples showed that the magnetic Bragg peak intensity of the SDW state is suppressed on entering the superconducting state, for x = 0.04 and 0.047. This certainly shows a very strong interaction between the superconducting and SDW states.It could be interpreted that this suppression is due to the same electrons participating in both the SDW and superconductivity favoring a phase coexistence scenario.However, in a phase separation scenario, a proximity effect could cause the superconducting regions to interfere with the SDW regions causing a reduction in the SDW volume consistent with the observed Bragg peak intensity reduction. Hence, it is difficult to make any strong conclusions about the implications of this observation for the question of phase coexistence.Interestingly, the details of the phase diagram in the region where the structural and magnetic transitions cross the superconducting dome have recently been explored with high resolution x-ray diffraction.

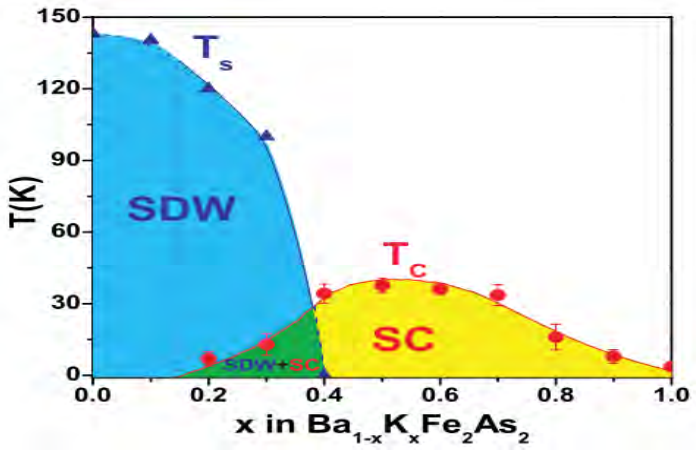

Figure 2.9: The composition-temperature phase diagram, showing the structural, magnetic and superconducting transitions.T_S denotes the temperature of the simultaneous structural and magnetic transition, and T_C the superconducting one.The spin-density wave (SDW) and superconducting (SC) orders coexist at low temperature for 0.2<x <0.4.[31]

The anomaly associated with the structural and magnetic transition is pronounced for x =0 and x=0.1.The anomaly is rounded off for x = 0.2, which becomes a superconductor with the transition starting at 14 K and the resistivity reaching zero at 3 K.The

T_C increases with further potassium doping and the superconducting transition becomes narrower until x = 0.5.Thereafter, T_C begins to decrease from the maximum $T_C = 37.5K$ with the increasing potassium doping. At x =1, T_C is 3.8 K for the KFe_2As_2 sample, the same as reported by Sasmal et al. [23]. The T_C as a function of the composition is summarized in fig. 3.While the temperature of the simultaneous structural and SDW transition can be inferred from the pronounced anomaly in resistivity for x = 0 and x=0.1 (fig. 2), for x= 0.2, it becomes progressively less certain whether there is an anomaly in the resistivity.To further investigate the crystal structure and structural transition, powder diffraction experiments from 5 to 300 K were performed for the x =0,0.1, 0.2, 0.3, 0.4 and 0.6 samples .

2.4 Mechanism of Pairing for superconductivity

The pairing mechanism in iron arsenides is currently in dispute.But even in these early days it becomes evident,that superconductivity in LaFeAsO emerges from specific structural and electronic conditions in the (FeAs) layer.However, if only the iron arsenide layer is essential, also other structure types could serve as parent compounds.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.Inconventional 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 Tc where the resistance also vanishes.For hightemperature superconductors this is more complicated since over the wide region of compositions and temperatures this energy gap exists quite well above the transitiontemperature and there is no relation between transition temperature and this energy gap.This is why this gap is called pseudogap.The origin of pseudogap 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 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 (32), NMR spectroscopy and high field resistivity measurement suggest the existence of unconventional superconductivity in these Fe based superconductors. The superconductivity emerging from these SDW compounds is theoretically proposed to be unconventional and mediated by AFM spin fluctuations.Such an SC state has an extended s-wave pairing with a sign reversal of the order parameter between different Fermi surface sheets, as the magnetic fluctuations, while too broad to induce a magnetic instability, are instrumental in stabilizing superconductivity (Chubukov et al. 2008; Kuroki et al. 2008; Mazin et al. 2008a,b).

2.4.1 Original Proposals forPairing

With the good nesting condition between the hole and electron pockets,it is natural to think that the electronic system will respond significantly with the AF SFs, especially when the AF vector matches nicely with the interpocket displacement.This interesting picture was firstproposed by Mazin et al.and later further formalized by several other groups using different theoretical approaches (33).More details about the pairing order parameter can be found in a recent review (34).

Two electrons on the electron (hole) FSs (marked with the thick arrows indicating opposite directions of spins) are scattered to the hole (electron) FSs by exchanging the AF SFs.If the pairing is really established through exchanging the AF SF, it is electronic in origin, and avoiding the strong repulsive interaction is actually the driving force for pairing.

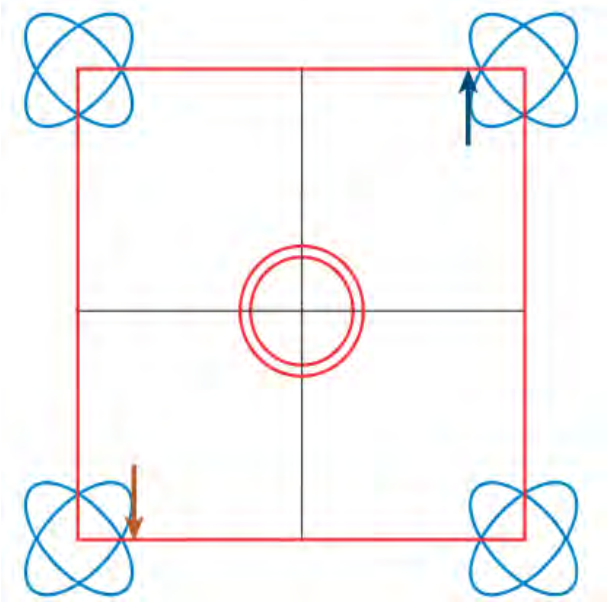

Figure 2.10: Fermi surfaces (FSs) and the interpocket electron scattering. The two electrons on the electron pockets, marked by the two arrows, are scattered to the hole pockets, or the two electrons on the hole pockets as marked by the red circles in the center of the Brillouin Zone (BZ), are scattered to the electron pockets.[33]

2.4.2 Anti-ferromagnetic spin fluctuation

Superconductivity emerging from these spindensity wave(SDW) compounds is theoretically proposed to be unconventional and mediated by antiferromagnetic spin fluctuation.Such superconducting state has an extended S-wave pairing with sign reversal of the order parameter between different Fermi surface (sheets) as the magnetic fluctuation while too broad to induce a magnetic instability are instrumental in stabilizing superconductivity.Any spin fluctuation induced interaction with this wave vector,nomatter what the origin of these fluctuation (Fermi-surface nesting,frustrated superexchange) or any thing else unavoidabily leads to a superconducting state with opposite signs of the order parameter for electrons and holes.Anti-ferromgnetism is relevant to high temperature superconductivity because copperoxide and Iron Arsenide superconductors arise from electron or hole doping of their anti-ferromagnetic parent compounds.There are two broad

class of explanation for anti-ferromagnetism, the first one is local moment picture appropriate for insulating copper oxide.For those systems anti-ferromagnetic interactions are well described by Heisenberg Hamiltonian whereas in the Itinerant model suitable for metallic Chromium ,anti-ferromagnetic order arises from quasiparticle excitations of nested Fermi surfaces. Spin fluctuations are the strongest candidate for the superconductivity and the models for spinfluctuations are based on the weak coupling itinerant limit with superconductivity related tothe presence of strong nesting between hole and electron sheets.

2.5 Phase transition and superconducting orderparameter

Phase transition can be classified in to broad catagories as follows Classifications

2.5.1 Ehrenfest classification

Paul Ehrenfest classified phase transitions based on the behavior of the thermodynamic free energy as a function of other thermodynamic variables.Under this scheme, phase transitions were labeled by the lowest derivative of the free energy that is discontinuous at the transition. First-order phase transitions exhibit a discontinuity in the first derivative of the free energy with respect tosome thermodynamic variable.The various solid/liquid/gas transitions are classified as first-order transitions because they involve a discontinuous change in density, which is the first derivative of the free energy with respect to chemical potential. Second-order phase transitions are continuous in the first derivative (the order parameter,which is the first derivative of the free energy with respect to the external field, is continuous across the transition) but exhibit discontinuity in a second derivative of the free energy. The include ferromagnetic phase transition in materials such as iron,

where the magnetization, which is the first derivative of the free energy with the applied magnetic field strength, increases continuously from zero as the temperature islowered below the Curie temperature. The magnetic susceptibility, the second derivative of the free energy with the field, changes discontinuously.Though useful, Ehrenfests classification has been found to be an inaccurate method of classifying phase transitions, for it does not take into account the case where a derivative of free energy diverges (which is only possible in thethermodynamic limit).For instance, in the ferromagnetic transition, the heat capacity diverges to infinity.

2.5.2 Modern classifications

In the modern classification scheme, phase transitions are divided into two broad categories, named similarly to the Ehrenfest classes:First-order phase transitions are those that involve a latent heat.During such a transition, a system either absorbs or releases a fixed (and typically large) amount of energy. During this process,the temperature of the system will stay constant as heat is added: the system is in a mixed-phase regime in which some parts of the system have completed the transition and others have not. Familiar examples are the melting of ice or the boiling of water (the water does not instantly turn into vapor, but forms a turbulent mixture of water and vapor bubbles).Second-order phase transitions are also called continuous phase transitions.They are characterized by a divergent susceptibility, an infinite correlation length, and a power-law decay of correlations near criticality.Examples of second-order phase transitions are the ferromagnetic transition, superconductor and the superfluid transition.Lev Landau gave a phenomenological theory ofsecond order phase transitions.

Chapter 3

Mathematical Method

3.1 Green's Function Formalism

The study of Green's function formalism provided the necessary background for understanding the significance of a modern useful tool, quantum field theory. With its success in elementary particle physics, it was shown to provide a powerful and unified way of solving the many body problem. In this thesis, we shall be mainly concerned with the quantum field theoretic technique known as the propagator or Green Function Theory (GFT). This is based on the idea that in order to find the important physical properties of a system it is not necessary to know the detailed behaviour of each particle but, rather, just the average behaviour of one or two typical particles. The quantities which describe this average behaviour are called the single particle propagator and two particle propagator, respectively.[35]

Following is the definition of a double -time ,retarded Green's function (propagators) for any two time dependent operators$\hat{A}(t)$ and $\hat{B}(t')$.

$$G^R(t,t') = \langle\langle \hat{A}(t)|\hat{B}(t')\rangle\rangle = -i\theta(t-t')\langle[\hat{A}(t),\hat{B}(t')]_{-\Omega}\rangle \tag{3.1.1}$$

with

$$[\hat{A}(t),\hat{B}(t')]_{-\Omega} = \hat{A}(t)\hat{B}(t') - \Omega\hat{B}(t')\hat{A}(t) \tag{3.1.2}$$

where we have used the following terminiologies :(R) means retarded ($t>t'$),$\theta(t-t')$ is the well known Heaviside step function while Ω= - for Fermions (satisfying canonical anticommutator relation[CAR] and Ω= + for Bosons (satisfying cannonical commutator relation[CCR].

The Green function $G^R(t,t')$ obeys the differential via the so called equation of motion method producing higher order Green functions which contain more operators compared to $G^R(t,t')$.

These higher order Green function when solved with in equation of motion method produces even higher order Green function .

This means that one has to deal with an infinite hierarchy to coupled differential equations.

In practice , one usually breaks it by making some approximation (decoupling procedure) in the lowest order of the eq.(3.1.1) and simply dropping all the other equations in the chain.

In the following we set up the equation of the motion of the retarded Green function while the same analysis for other types of Green's function (advanced, casual). We differentiate the definitions eq(3.1.1) and eq(3.1.2) with respect to t and make use of the following equations for any general operators $\hat{A}(t)$.

$$i\hbar\frac{d}{dt}\hat{A}(t) = [\hat{A}(t), \hat{H}] \tag{3.1.3}$$

then obtain

$$i\frac{d}{dt}G^R(t,t') = \frac{d}{dt}\theta(t-t')\langle[\hat{A}(t), \hat{B}(t')]_{-\Omega}\rangle + \langle\langle i\frac{d}{dt}\hat{A}(t)|\hat{B}(t')\rangle\rangle \tag{3.1.4}$$

$$i\frac{d}{dt}\langle\langle\hat{A}(t)|\hat{B}(t')\rangle\rangle^{(R)} = \delta(t-t')\langle[\hat{A}(t)|\hat{B}(t')]_{-\Omega}\rangle + \langle\langle[\hat{A}(t), \hat{H}]_{-}|\hat{B}(t')\rangle\rangle^{(R)} \tag{3.1.5}$$

where we have assumed that $\hbar$=1 and it has remained through out the whole thesis.

We have also made use of the following relation between the discontinous Heaviside function and delta function.

$$\theta(t) = \int_{-\infty}^{t} \delta(t-t')dt \tag{3.1.6}$$
$$\delta(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega(t-t')}d\omega$$

The commmutator $[\hat{A}(t), \hat{H}]_-$ on the right will give Green functions which generally contain more operators than left.

The equation of the motion of these higher order Green function is

$$i\frac{d}{dt}\langle\langle[\hat{A}(t),\hat{H}]_-|\hat{B}(t')\rangle\rangle^{(R)} = \delta(t-t')\langle[[\hat{A}(t),\hat{H}]_-|\hat{B}(t')]_{-\Omega}\rangle + \langle\langle[[\hat{A}(t),\hat{H}]_-,\hat{H}]_-|\hat{B}(t')\rangle\rangle^{(R)} \tag{3.1.7}$$

Generally, the last term has again a higher order than the term on the left and has a new equation of motion and so on. Finally, one obtains an infinite chain of equations of the Green functions as discussed before and thus, one is forced upon using some kind of an approximation. But before doing so it is useful to calculate the Fourier transform of $\langle\langle\hat{A}(t)|\hat{B}(t')\rangle\rangle^R$

$$\langle\langle\hat{A}|\hat{B}\rangle\rangle_\omega^R = \int_{-\infty}^{\infty}\langle\langle\hat{A}(t)|\hat{B}(t')\rangle\rangle^R e^{i\omega(t-t')}d(t-t') \tag{3.1.8}$$

because then we obtain ordinary equations instead of differential equations i.e.

$$\omega\langle\langle\hat{A}|\hat{B}\rangle\rangle_\omega^R = \langle[\hat{A}|\hat{B}]_{-\Omega}\rangle + \langle\langle[\hat{A},\hat{H}]_-|\hat{B}\rangle\rangle_\omega^R \tag{3.1.9}$$

The simplest approximation of the Green function is obtained if one can convert the term $\langle\langle[\hat{A},\hat{H}]_-|\hat{B}\rangle\rangle$

to the form

$$G^R(\omega) = \langle\langle\hat{A},\hat{B}\rangle\rangle_\omega^R = \frac{\langle[\hat{A},\hat{B}]_{-\Omega}\rangle}{\{\omega - P(\omega)\}} \tag{3.1.10}$$

Now if we consider $\hat{A} = C_{ij\sigma}$ and $\hat{B} = C_{ij\sigma}^\dagger$, where are $C_{ij\sigma}$and$C_{ij\sigma}^\dagger$

are anni-hilation and creation operators of an electron respectively, then we can define the corresponding single particle or one electron Green function:

$$G^{(R)}_{ij\sigma}(\omega) = \langle\langle C_{ij\sigma}|C^{\dagger}_{ij\sigma}\rangle\rangle^{(R)}_{\omega} \tag{3.1.11}$$

and its Fourier transform

$$G^{R}_{k\sigma}(\omega) = \frac{1}{N}\sum_{ij} G_{ij,\sigma^{R}(\omega)} e^{-ik.(R_i - R_j)} \tag{3.1.12}$$

CAR algebra and Fourier transforms

In this thesis, we make use of the following canonical anti- commutation relations (CAR) algebra:

$$\{C_{i\alpha\sigma}, C_{j\beta\sigma'}\} = \{C^{\dagger}_{i\alpha\sigma}, C^{\dagger}_{j\beta\sigma\sigma'}\} = 0 \tag{3.1.13}$$

$$\{C_{i\alpha\sigma}, C^{\dagger}_{j\beta\sigma'}\}_{+} = \delta_{ij}\delta_{\alpha\beta}\delta_{\sigma\sigma'} \tag{3.1.14}$$

$$\{C_{i\alpha\sigma}, n^{\dagger}_{j\beta\sigma'}\}_{-} = \delta_{ij}\delta_{\alpha\beta}\delta_{\sigma\sigma'}C_{i\alpha\sigma} \tag{3.1.15}$$

where

$$n_{j\beta\sigma'} = C^{\dagger}_{j\beta\sigma'}C_{j\beta\sigma'}$$

Commutators and operator Algebra(Bosonic operators)

The commmutator $[A, B]$ $=AB - BA$ of two operators plays a prominant role in quantum mechanics. The most important commutators are those involving cannonically conjugate variables , such as position and momentum, energy and time , angular momentum and angular displacement. The manipulation of commutation relations for various dynamical variables as Dirac called the operators that represent physical quantities is most safely accomplished by allowing the operators to act on arbitrary function. In commutator bracket notation , for any operators the following elementary rules are easy to verify

$[A, B] + [B, A]$=0

$[A, A]$=0

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

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

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

Anti-commutation relation(Fermionic operators)

$\{A + B, C\} = \{A, C\} + \{B, C\}$

$\{AB, C\} = A\{B, C\} + \{A, C\}B$

$\{A, BC\} = \{A, B\}C + B\{A, C\}$

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

The value of some parameters we have used in this thesis are the following $\hbar\omega \approx 13 \times 10^{-3} ev$,$\lambda \approx 0.272$

Chapter 4

Theoretical Formulation

4.1 Model Hamiltonian

This formulation is the most fundamental techniques that lead the experimentalists to check its feseability using mathematical models.Here particularly the model we used to formulate Green's function for free electrons, superconducting electrons and the spin density wave is Hamiltonian.Theoretical formulation is used to relate energy gap(order parameter) with the superconducting and spin density wave transition temperature.We use the following Model Hamiltonian for our system.

$$H = H_o + H_I + H_{sdw}$$

$$H = \sum_{k'\sigma'} \epsilon_{k'} C^{\dagger}_{k'\sigma'} C_{k'\sigma'} + \Delta_1 \sum_{k'} \{C^{\dagger}_{k'} \uparrow C^{\dagger}_{-k'} \downarrow + C_{-k'} \downarrow C_{k'} \uparrow\} + \Delta_2 \sum_{k',Q} \{C^{\dagger}_{k'+Q} \uparrow C_{k'} \downarrow + C^{\dagger}_{k'} \downarrow C_{k'+Q} \uparrow\} \tag{4.1.1}$$

where

$$H_o = \sum_{k'\sigma'} \epsilon_{k'} C^{\dagger}_{k'\sigma'} C_{k'\sigma'}$$

$$H_I = \Delta_1 \sum_{k'} \{C^{\dagger}_{k'} \uparrow C^{\dagger}_{-k'} \downarrow + C_{-k'} \downarrow C_{k'} \uparrow\}$$

$$H_{sdw} = \Delta_2 \sum_{k',Q} \{C^{\dagger}_{k'+Q} \uparrow C_{k'} \downarrow + C^{\dagger}_{k'} \downarrow C_{k'+Q} \uparrow\}$$

$$\Delta_1 = -\sum_{k'} V(k,k')\langle C_{k'} \uparrow C_{-k'} \downarrow\rangle$$

$$\Delta_2 = -U\sum_{k',Q}\langle C^{\dagger}_{k'} \uparrow C_{k'-Q} \downarrow\rangle$$

Where $C^{\dagger}_{k'\sigma'}(C_{k'\sigma'})$ are creation(annihilation) Fermionic operators.

4.2 Equation of motion

Physical observables can be expressed interms of retarded Green's function and correlation functions .In many cases we need to calculate the time dependence of these functions.There are several ways of solving this 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 correlation function at hand a number of times.

Formulating the Green's function for the above Hamiltonian ,we will have the following

Now we define

$$G^{\uparrow\uparrow}_{k'k} = \langle\langle C_k \uparrow | C^{\dagger}_{k'} \uparrow\rangle\rangle$$

Let $\Delta_{SC} = \Delta_1$ and $\Delta_{SDW} = \Delta_2$

$$\omega\langle\langle C_k \uparrow | C^{\dagger}_{k'} \uparrow\rangle\rangle_{\omega} = \langle[C_k \uparrow, C^{\dagger}_{k'} \uparrow]\rangle + \langle\langle[C_k, \hat{H}]| C^{\dagger}_{k'} \uparrow\rangle\rangle_{\omega} \tag{4.2.1}$$

Applying the anti-commutation relation for creation(annihilation)operators i.e

$[A, BC]$=$\{A, B\}C - B\{A, C\}$, we will have the following:

For free electron

$$[C_k \uparrow, H_o] = [C_k \uparrow, \sum_{k'\sigma'} \epsilon_{k'} C^{\dagger}_{k'\sigma'} C_{k'\sigma'}] = \sum_{k'} \epsilon_{k'}\{C_k \uparrow, C^{\dagger}_{k'\sigma'}\}C_{k'\sigma'} = \sum_{k'} \epsilon_{k'}\delta_{kk'}\delta_{\sigma\sigma'}C_{k'\sigma'} = \epsilon_k C_k \uparrow \tag{4.2.2}$$

For superconducting part

$$[C_k \uparrow, H_I] = [C_k \uparrow, \Delta_1 \sum_{k'}(C^{\dagger}_{k'} \uparrow C^{\dagger}_{-k'} \downarrow + C_{-k'} \downarrow C_{k'} \uparrow)]$$

$$= \Delta_1 \Big\{ \sum_{k'} \{C_k \uparrow, C^\dagger_{k'} \uparrow C^\dagger_{-k'} \downarrow\} \Big\} = \Delta_1 \Big\{ \sum_{k'} \{C_k \uparrow, C^\dagger_{k'} \uparrow\} C^\dagger_{-k'} \downarrow \Big\} = \Delta_1 \Big\{ \sum_{k'} \delta_{kk'} \delta \uparrow\uparrow C^\dagger_{-k'} \downarrow \Big\} \tag{4.2.3}$$

$$= \Delta_1 C^\dagger_{-k} \downarrow$$

For SDW part

$$[C_k \uparrow, H_{sdw}] = [C_k \uparrow, \Delta_2 \sum_{k',Q} (C^\dagger_{k'+Q} \uparrow C_{k'} \downarrow + C^\dagger_{k'} \downarrow C_{k'+Q} \uparrow)] = \Delta_2 \sum_{k',Q} \{C_k \uparrow, C^\dagger_{k'+Q} \uparrow C_{k'} \downarrow\} \tag{4.2.4}$$

$$= \Delta_2 \sum_{k',Q} \{C_k \uparrow, C^\dagger_{k'+Q} \uparrow C_{k'} \downarrow\} = \Delta_2 \sum_{k',Q} \delta_{k(k'+Q)} \delta_{\uparrow\uparrow} C_{k'} \downarrow = \Delta_2 C_{k-Q} \downarrow$$

using the eq(4.2.1),we can write the equation of motion for eq(4.2.2),eq(4.2.3) and eq(4.2.4) as follows

$$(\omega - \epsilon_k) \langle\langle C_k \uparrow | C^\dagger_k \uparrow \rangle\rangle_\omega = 1 + \Delta_1 \langle\langle C^\dagger_{-k} \downarrow | C^\dagger_k \uparrow \rangle\rangle_\omega + \Delta_2 \langle\langle C_{k-Q} \downarrow | C^\dagger_k \uparrow \rangle\rangle_\omega \tag{4.2.5}$$

$$G^{\downarrow\uparrow}_{k(-k)} = \langle\langle C^\dagger_{-k} \downarrow | C^\dagger_{k'} \uparrow \rangle\rangle$$

For free electron

$$[C^\dagger_{-k} \downarrow, \sum_{k'\sigma'} \epsilon_{k'} C^\dagger_{k'\sigma'} C_{k'\sigma'}] = -\sum_{k'\sigma'} \epsilon_{k'} C^\dagger_{k'\sigma'} \{C^\dagger_{-k} \downarrow, C_{k'\sigma'}\} = \sum_{k'\sigma'} \epsilon_{k'} \delta_{(-k)k'} \delta_{\sigma\sigma'} C_{k'\sigma'} = -\epsilon_k C^\dagger_{-k} \downarrow \tag{4.2.6}$$

For superconducting part

$$[C^\dagger_{-k} \downarrow, \Delta_1 \sum_{k'} \{C^\dagger_{k'} \uparrow C^\dagger_{-k'} \downarrow + C_{-k'} \downarrow C_{k'} \uparrow\}] = \Delta_1 \sum_{k'} (\{C^\dagger_{-k} \downarrow, C_{-k'} \downarrow\} C_{k'} \downarrow\uparrow) \tag{4.2.7}$$

$$= \Delta_1 \sum_{k'} \delta_{-kk'} \delta_{\downarrow\downarrow} C_k \uparrow = \Delta_1 C_k \uparrow$$

For SDW part

$$[C^\dagger_{-k} \downarrow, \Delta_2 \sum_{k',Q} (C^\dagger_{k'+Q} \uparrow C_{k'} \downarrow + C^\dagger_{k'} \downarrow C_{k'+Q} \uparrow)] = \Delta_2 \sum_{k',Q} C^\dagger_{k'+Q} \uparrow \{C^\dagger_{-k} \downarrow, C_{k'} \downarrow\} \tag{4.2.8}$$

$$= -\Delta_2 \sum_{k'} \delta_{-k(k')} \delta_{\downarrow\downarrow} C^{\dagger}_{k'+Q} \uparrow = -\Delta_2 C^{\dagger}_{-k+Q} \uparrow$$

after transforming the above Green's function the equation of motion becomes

$$(\omega + \epsilon_k)\langle\langle C^{\dagger}_{-k} \downarrow | C^{\dagger}_{k} \uparrow\rangle\rangle = \Delta_1 \langle\langle C_k \uparrow | C^{\dagger}_{k} \uparrow\rangle\rangle - \Delta_2 \langle\langle C^{\dagger}_{-k+Q} \uparrow | C^{\dagger}_{k} \uparrow\rangle\rangle \tag{4.2.9}$$

$$G^{\downarrow\uparrow}_{(k-Q)k'} = \langle\langle C_{k-Q} \downarrow | C^{\dagger}_{k'}\rangle\rangle$$

For free electron

$$[C_{k-Q} \downarrow, (\sum_{k'\sigma'} \epsilon_{k'} C^{\dagger}_{k'\sigma'} C_{k'\sigma'}] = \sum_{k'\sigma'} \epsilon_{k'} (\{C_{k-Q} \downarrow, C^{\dagger}_{k'\sigma'}\} C_{k'\sigma'}) = \sum_{k'} \epsilon_{k'} \delta_{(k-Q)k'} \delta_{\sigma\sigma'} C_{k'\sigma'} = \epsilon_{k-Q} C_{k-Q} \downarrow \tag{4.2.10}$$

For supconducting part

$$[C_{k-Q} \downarrow, \Delta_1 \sum_{k'} (C^{\dagger}_{k'} \uparrow C^{\dagger}_{-k'} \downarrow + C_{-k'} \downarrow C_{k'} \uparrow)] = -\Delta_1 \sum_{k'} \{C_{k-Q} \downarrow, C^{\dagger}_{k'} \uparrow C^{\dagger}_{-k'} \downarrow \tag{4.2.11}$$

$$-\Delta_1 \sum_{k'} \delta_{(k-Q)k'} \delta \downarrow\downarrow C^{\dagger}_{k'} \uparrow = -\Delta_1 C^{\dagger}_{-k+Q} \uparrow$$

For SDW

$$[C_{k-Q} \downarrow, \Delta_2 \sum_{k',Q} \{C^{\dagger}_{k'+Q} \uparrow C_{k'} \downarrow + C^{\dagger}_{k'} \downarrow C_{k'+Q} \uparrow\} = \Delta_2 \sum_{k',Q} (\{C_{k-Q} \downarrow, C^{\dagger}_{k'} \downarrow C_{k'+Q} \uparrow\} \tag{4.2.12}$$

$$= \Delta_2 \sum_{k',Q} \{C_{k-Q} \downarrow, C^{\dagger}_{k'} \downarrow\} C_{k'+Q} \uparrow = \Delta_2 \sum_{k',Q} \delta_{(k-Q)k'} \delta_{\downarrow\downarrow} C_{k'+Q} \uparrow = \Delta_2 C_k \uparrow$$

equation of motion

$$(\omega - \epsilon_{k-Q})\langle\langle C_{k-Q} \downarrow | C^{\dagger}_{k}\rangle\rangle = -\Delta_1 \langle\langle C^{\dagger}_{-k+Q} \uparrow | C^{\dagger}_{k} \uparrow\rangle\rangle + \Delta_2 \langle\langle C_k \uparrow | C^{\dagger}_{k} \uparrow\rangle\rangle \tag{4.2.13}$$

$$G^{\uparrow\uparrow}_{(-k+Q)k'} = \langle\langle C^{\dagger}_{-k+Q} \uparrow | C^{\dagger}_{k} \uparrow\rangle\rangle$$

For free electron

$$[C^{\dagger}_{-k+Q} \uparrow, (\sum_{k'\sigma'} \epsilon_{k'} C^{\dagger}_{k\sigma'} C_{k'\sigma'})] = -\sum_{k'\sigma'} C^{\dagger}_{k'\sigma'} \{C^{\dagger}_{-k+Q} \uparrow, C_{k'\sigma'}\} = -\sum_{k'} \epsilon_{k'} \delta_{(-k+Q)k'} \delta_{\sigma\sigma'} C^{\dagger}_{k'\sigma'} \tag{4.2.14}$$

$$= -\epsilon_{-k+Q} C^{\dagger}_{-k+Q} \uparrow = -\epsilon_{k-Q} C^{\dagger}_{-k+Q} \uparrow$$

For superconducting part

$$[C^{\dagger}_{-k+Q}\uparrow, \Delta_1 \sum_k (C^{\dagger}_{k'}\uparrow C^{\dagger}_{-k'}\downarrow + C_{-k'}\downarrow C_{k'}\uparrow)] = \Delta_1 \sum_{k'\sigma'} \{C^{\dagger}_{-k+Q}\uparrow, C_{-k'}\downarrow C_{k'}\uparrow\}\} \tag{4.2.15}$$

$$= -\Delta_1 \sum_{k'} C_{-k'}\downarrow \{C^{\dagger}_{-k+Q}\uparrow, C^{\dagger}_{k'}\uparrow\} = -\Delta_1 \sum_{k'} \delta_{(-k+Q)k'}\delta_{\uparrow\uparrow} C_{-k'}\downarrow = -\Delta_1 C_{k-Q}\downarrow$$

For SDW

$$[C^{\dagger}_{-k+Q}\uparrow, \Delta_2 \sum_{k',Q} \{C^{\dagger}_{k'+Q}\uparrow C_{k'}\downarrow + C^{\dagger}_{k'}\downarrow C_{k'+Q}\uparrow\}] = -\Delta_2 \sum_{k',Q} C^{\dagger}_{k'}\downarrow \{C^{\dagger}_{-k+Q}\uparrow, C_{k'+Q}\uparrow\} \tag{4.2.16}$$

$$= -\Delta_2 \sum_{k'} C^{\dagger}_{k'}\downarrow \{C^{\dagger}_{-k+Q}\uparrow, C_{k'+Q}\uparrow\} = -\Delta_2 \sum_{k'} \delta_{(-k+Q)k'}\delta_{\uparrow\uparrow} C^{\dagger}_{k'}\downarrow = -\Delta_2 C^{\dagger}_{-k}\downarrow$$

Equation of motion

$$(\omega + \epsilon_{k-Q})\langle\langle C^{\dagger}_{-k+Q}\uparrow | C^{\dagger}_{k}\uparrow\rangle\rangle = -\Delta_1 \langle\langle C_{(k-Q)}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle - \Delta_2 \langle\langle C^{\dagger}_{-k}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle \tag{4.2.17}$$

From eq(4.2.5),eq(4.2.9),eq(4.2.13) and eq(4.2.17),we will obtain the following relation

$$\langle\langle C_k\uparrow | C^{\dagger}_{k}\uparrow\rangle\rangle = \frac{1}{\omega - \epsilon_k}\left\{1 + \Delta_1 \langle\langle C^{\dagger}_{-k}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle + \Delta_2 \langle\langle C_{k-Q}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle\right\} \tag{4.2.18}$$

$$\langle\langle C^{\dagger}_{-k}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle = \frac{1}{\omega + \epsilon_k}\left\{\Delta_1 \langle\langle C_k\uparrow | C^{\dagger}_{k}\uparrow\rangle\rangle - \Delta_2 \langle\langle C^{\dagger}_{-k+Q}\uparrow | C^{\dagger}_{k}\uparrow\rangle\rangle\right\} \tag{4.2.19}$$

$$\langle\langle C_{k-Q}\downarrow | C^{\dagger}_{k}\rangle\rangle = \frac{1}{\omega - \epsilon_{k-Q}}\left\{ - \Delta_1 \langle\langle C^{\dagger}_{-k+Q}\uparrow | C^{\dagger}_{k}\uparrow\rangle\rangle + \Delta_2 \langle\langle C_k\uparrow | C^{\dagger}_{k}\uparrow\rangle\rangle\right\} \tag{4.2.20}$$

$$\langle\langle C^{\dagger}_{-k+Q}\uparrow | C^{\dagger}_{k}\uparrow\rangle\rangle = \frac{-1}{\omega + \epsilon_{k-Q}}\left\{\Delta_1 \langle\langle C_{k-Q}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle + \Delta_2 \langle\langle C^{\dagger}_{-k}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle\right\} \tag{4.2.21}$$

substituting eq(4.2.18)and eq(4.2.21) into eq(4.2.19) ,we will obtain the relation

$$\langle\langle C^{\dagger}_{-k}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle = \frac{\Delta_1}{\omega^2 - \epsilon_k^2} + \left\{\frac{\Delta_1^2}{\omega^2 - \epsilon_k^2} + \frac{\Delta_2^2}{(\omega - \epsilon_k)(\omega + \epsilon_{k-Q})}\right\}\langle\langle C^{\dagger}_{-k}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle$$

$$+\left\{\frac{\Delta_1\Delta_2}{\omega^2 - \epsilon_k^2} + \frac{\Delta_1\Delta_2}{(\omega + \epsilon_k)(\omega + \epsilon_{k-Q})}\right\}\langle\langle C_{k-Q}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle \tag{4.2.22}$$

$$\langle\langle C^{\dagger}_{-k}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle = \frac{\Delta_1}{\omega^2 - \epsilon_k^2} + \left\{\frac{\Delta_1^2(\omega + \epsilon_{k-Q}) + \Delta_2^2(\omega - \epsilon_k)}{(\omega^2 - \epsilon_k^2)(\omega + \epsilon_{k-Q})}\right\}\langle\langle C^{\dagger}_{-k}\downarrow | C^{\dagger}_{k}\uparrow\rangle\rangle \tag{4.2.23}$$

$$+\left\{\frac{\Delta_1\Delta_2(\omega+\epsilon_{k-Q}+\omega-\epsilon_k)}{(\omega^2-\epsilon_k^2)(\omega+\epsilon_{k-Q})}\right\}\langle\langle C_{k-Q}\downarrow|C_k^\dagger\uparrow\rangle\rangle$$

$$\langle\langle C_{-k}^\dagger\downarrow|C_k^\dagger\uparrow\rangle\rangle-\frac{\Delta_1\Delta_2(\omega+\epsilon_{k-Q}+\omega-\epsilon_k)}{(\omega^2-\epsilon_k^2)(\omega+\epsilon_{k-Q})-\{\Delta_1^2(\omega+\epsilon_{k-Q})+\Delta_2^2(\omega-\epsilon_k)\}}\langle\langle C_{k-Q}\downarrow|C_k^\dagger\uparrow\rangle\rangle \tag{4.2.24}$$

$$=\frac{\Delta_1(\omega+\epsilon_{k-Q})}{(\omega^2-\epsilon_k^2)(\omega+\epsilon_{k-Q})-\{\Delta_1^2(\omega+\epsilon_{k-Q})+\Delta_2^2(\omega-\epsilon_k)\}}$$

Similarly by substituting eq(4.2.18) and eq(4.2.21) into eq(4.2.20), we will obtain

$$\langle\langle C_{k-Q}\downarrow|C_k^\dagger\uparrow\rangle\rangle=\left\{\frac{\Delta_1^2}{\omega^2-\epsilon_{k-Q}^2}+\frac{\Delta_2^2}{(\omega-\epsilon_k)(\omega-\epsilon_{k-Q})}\right\}\langle\langle C_{k-Q}\downarrow|C_k^\dagger\uparrow\rangle\rangle+\frac{\Delta_2}{(\omega-\epsilon_{k-Q})(\omega-\epsilon_k)}$$

$$+\Delta_1\Delta_2\left\{\frac{1}{\omega^2-\epsilon_{k-Q}^2}+\frac{1}{(\omega-\epsilon_k)(\omega-\epsilon_{k-Q})}\right\}\langle\langle C_{-k}^\dagger\downarrow|C_k^\dagger\uparrow\rangle\rangle \tag{4.2.25}$$

rearranging the above expression , we will obtain the following relation

$$\frac{-\Delta_1\Delta_2(\omega-\epsilon_k+\omega+\epsilon_{k-Q})}{(\omega^2-\epsilon_{k-Q}^2)(\omega-\epsilon_k)-\{\Delta_1^2(\omega-\epsilon_k)+\Delta_2^2(\omega+\epsilon_{k-Q})\}}\langle\langle C_{-k}^\dagger\downarrow|C_k^\dagger\uparrow\rangle\rangle+\langle\langle C_{k-Q}\downarrow|C_k^\dagger\uparrow\rangle\rangle$$

$$=\frac{\Delta_2(\omega+\epsilon_{k-Q})}{(\omega^2-\epsilon_{k-Q}^2)(\omega-\epsilon_k)-\{\Delta_1^2(\omega-\epsilon_k)+\Delta_2^2(\omega+\epsilon_{k-Q})\}} \tag{4.2.26}$$

Let us take some approximation

$$\frac{\omega+\epsilon_{k-Q}}{\omega-\epsilon_k}\approxeq 1$$

Define

$$\beta=(\omega^2-\epsilon_{k-Q}^2)(\omega-\epsilon_k)-\{\Delta_1^2(\omega-\epsilon_k)+\Delta_2^2(\omega+\epsilon_{k-Q})\}$$

$$\alpha=(\omega+\epsilon_{k-Q}+\omega-\epsilon_k)$$

The solution for eq(4.2.24) and eq(4.2.26) can be solved using the matrices method as follows

Let M and R be the matrices representation of the system of linear equations given above

$$M=\begin{pmatrix}1 & \frac{-\alpha\Delta_1\Delta_2}{\beta}\\ \frac{-\alpha\Delta_1\Delta_2}{\beta} & 1\end{pmatrix} \tag{4.2.27}$$

$$R = \begin{pmatrix} \frac{\Delta_1(\omega+\epsilon_{k-Q})}{\beta} \\ \frac{\Delta_2(\omega+\epsilon_{k-Q})}{\beta} \end{pmatrix} \tag{4.2.28}$$

the determinant of the matrix M is given by

$$\det M = ||M|| = \begin{vmatrix} 1 & \frac{-\alpha\Delta_1\Delta_2}{\beta} \\ \frac{-\alpha\Delta_1\Delta_2}{\beta} & 1 \end{vmatrix} = \frac{\beta^2 - (\alpha\Delta_1\Delta_2)^2}{\beta^2} \tag{4.2.29}$$

to determine the value of $\langle\langle C^\dagger_{-k} \downarrow | C^\dagger_k \uparrow\rangle\rangle$ substitute the first column of matrix M by the column matrix R and find the determinant of the new matrix .LetM_1 be the new matrix representing the matrix elements.

$$M_1 = \begin{pmatrix} \frac{\Delta_1(\omega+\epsilon_{k-Q})}{\beta} & \frac{-\alpha\Delta_1\Delta_2}{\beta} \\ \frac{\Delta_2(\omega+\epsilon_{k-Q})}{\beta} & 1 \end{pmatrix} \tag{4.2.30}$$

then the determinant of new matrix becomes

$$\det M_1 = ||M_1|| = \begin{vmatrix} \frac{\Delta_1(\omega+\epsilon_{k-Q})}{\beta} & \frac{-\alpha\Delta_1\Delta_2}{\beta} \\ \frac{\Delta_2(\omega+\epsilon_{k-Q})}{\beta} & 1 \end{vmatrix} = \frac{\beta\Delta_1(\omega+\epsilon_{k-Q}) + \alpha\Delta_1\Delta_2^2(\omega+\epsilon_{k-Q})}{\beta^2} \tag{4.2.31}$$

Then

$$\langle\langle C^\dagger_{-k} \downarrow | C^\dagger_k \uparrow\rangle\rangle = \frac{\det M_1}{\det M} = \frac{\beta\Delta_1(\omega+\epsilon_{k-Q}) + \alpha\Delta_1\Delta_2^2(\omega+\epsilon_{k-Q})}{\beta^2 - (\alpha\Delta_1\Delta_2)^2} \tag{4.2.32}$$

$$\langle\langle C^\dagger_{-k} \downarrow | C^\dagger_k \uparrow\rangle\rangle = \frac{\beta\Delta_1(\omega+\epsilon_{k-Q}) + \alpha\Delta_1\Delta_2^2(\omega+\epsilon_{k-Q})}{(\beta - \alpha\Delta_1\Delta_2)(\beta + \alpha\Delta_1\Delta_2)}$$

$$\langle\langle C^\dagger_{-k} \downarrow | C^\dagger_k \uparrow\rangle\rangle = \frac{\beta\Delta_1(\omega+\epsilon_{k-Q}) + \Delta_1\Delta_2^2(\omega+\epsilon_{k-Q})\alpha}{(\beta - \alpha\Delta_1\Delta_2)(\beta + \alpha\Delta_1\Delta_2)} \tag{4.2.33}$$

after simplifying eq(4.2.33) , we can rewrite as

$$\langle\langle C^\dagger_{-k} \downarrow | C^\dagger_k \uparrow\rangle\rangle = \frac{\Delta_1\{(\omega-\epsilon_k) - (\Delta_1^2 + \Delta_2^2)\} + 2\Delta_1\Delta_2^2}{\{(\omega^2 - \epsilon_k^2) - (\Delta_1 + \Delta_2)^2\}\{(\omega^2 - \epsilon_k^2) - (\Delta_1 - \Delta_2)^2\}} \tag{4.2.34}$$

Using the method of partial fraction, we can decouple eq(4.2.34) and write as the sum of ratio of two separate fractions.Suppose that A and B are functions of order parameters which can be given by the relation

$$A = M(\Delta_1 \mp \Delta_2) + Q$$

$$B = N(\Delta_1 \pm \Delta_2) + P \tag{4.2.35}$$

$$\frac{A}{(\omega^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2}+\frac{B}{(\omega^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2} = \frac{\Delta_1\{(\omega-\epsilon_k)-(\Delta_1^2+\Delta_2^2)\}+2\Delta_1\Delta_2^2}{\{(\omega^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2\}\{(\omega^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2} \tag{4.2.36}$$

$$A\{(\omega^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2\}+B\{(\omega^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2\} = \Delta_1\{(\omega-\epsilon_k)-(\Delta_1^2+\Delta_2^2)\}+2\Delta_1\Delta_2^2 \tag{4.2.37}$$

$$\{A+B\}(\omega^2-\epsilon_k^2)-A\{(\Delta_1-\Delta_2)^2\}-B\{(\Delta_1+\Delta_2)^2\} = \Delta_1\{(\omega-\epsilon_k)-(\Delta_1^2+\Delta_2^2)\}+2\Delta_1\Delta_2^2$$

$$-(A+B)(\Delta_1^2+\Delta_2^2) = -\Delta_1(\Delta_1^2+\Delta_2^2) \tag{4.2.38}$$

$$A + B = \Delta_1$$

$$2\Delta_1\Delta_2(A-B) = 2\Delta_1\Delta_2^2 \tag{4.2.39}$$

$$A - B = \Delta_2$$

solving eq(4.2.38) and eq(4.2.39) simultaneously

$$A = \frac{\Delta_1+\Delta_2}{2}$$

$$B = \frac{\Delta_1-\Delta_2}{2}$$

substituting this result in eq(4.2.36),we will get the the following:

$$\langle\langle C_{-k}^\dagger \downarrow | C_k^\dagger \uparrow\rangle\rangle = \frac{1}{2}\left\{\frac{\Delta_1+\Delta_2}{(\omega^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2}+\frac{\Delta_1-\Delta_2}{(\omega^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2}\right\} \tag{4.2.40}$$

Similarly, we can solve for

$$\langle\langle C_{k-Q} \downarrow | C_k^\dagger \uparrow\rangle\rangle$$

substituting the second column of matrix M by the column matrix R and determine the determinant of the new matrix:

$$M_2 = \begin{pmatrix} 1 & \frac{\Delta_1(\omega+\epsilon_{k-Q})}{\beta} \\ \frac{-\alpha\Delta_1\Delta_2}{\beta} & \frac{\Delta_2(\omega+\epsilon_{k-Q})}{\beta} \end{pmatrix} \tag{4.2.41}$$

$$\det M_2 = ||M_2|| = \begin{vmatrix} 1 & \frac{\Delta_1(\omega+\epsilon_{k-Q})}{\beta} \\ \frac{-\alpha\Delta_1\Delta_2}{\beta} & \frac{\Delta_2(\omega+\epsilon_{k-Q})}{\beta} \end{vmatrix} = \frac{\beta\Delta_2(\omega+\epsilon_{k-Q})+\alpha\Delta_1^2\Delta_2(\omega+\epsilon_{k-Q})}{\beta^2} \tag{4.2.42}$$

$$\langle\langle C_{k-Q}\downarrow|C_k^\dagger\uparrow\rangle\rangle = \frac{\det M_1}{\det M} = \frac{\beta\Delta_2(\omega+\epsilon_{k-Q}) + \alpha\Delta_1^2\Delta_2(\omega+\epsilon_{k-Q})}{\beta^2-(\alpha\Delta_1\Delta_2)^2} \tag{4.2.43}$$

$$\langle\langle C_{k-Q}\downarrow|C_k^\dagger\uparrow\rangle\rangle = \frac{\beta\Delta_2(\omega+\epsilon_{k-Q}) + \Delta_2\Delta_1^2(\omega+\epsilon_{k-Q})\alpha}{(\beta-\alpha\Delta_1\Delta_2)(\beta+\alpha\Delta_1\Delta_2)} \tag{4.2.44}$$

$$\langle\langle C_{k-Q}\downarrow|C_k^\dagger\uparrow\rangle\rangle = \frac{\Delta_2\{(\omega-\epsilon_k)-(\Delta_2^2+\Delta_1^2)\}+2\Delta_2\Delta_1^2}{\{(\omega^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2\}\{(\omega^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2\}} \tag{4.2.45}$$

Using the method of partial fraction, we can write the coupled equation separately , here A' and B' are functions of order parameters which may be given by the following relation

$$A' = M'(\Delta_1 \mp \Delta_2) + Q' \tag{4.2.46}$$

$$B' = N'(\Delta_1 \pm \Delta_2) + P'$$

$$\frac{\Delta_2\{(\omega-\epsilon_k)-(\Delta_2^2+\Delta_1^2)\}+2\Delta_2\Delta_1^2}{\{(\omega^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2\}\{(\omega^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2\}} = \frac{A'}{(\omega^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2} + \frac{B'}{(\omega^2-\epsilon_k^2)-(\Delta_1-\Delta_2)} \tag{4.2.47}$$

$$(A'+B')\{\omega^2-\epsilon_k^2\} - A'(\Delta_1-\Delta_2)^2 - B'(\Delta_1+\Delta_2)^2) = \Delta_2\{(\omega-\epsilon_k)-(\Delta_2^2+\Delta_1^2)\}+2\Delta_2\Delta_1^2 \tag{4.2.48}$$

equating terms from LHS with RHS consisting of the same order

$$-(A'+B')(\Delta_1^2+\Delta_2^2) = -\Delta_2(\Delta_1^2+\Delta_2^2) \tag{4.2.49}$$

from this

$$A'+B' = \Delta_2$$

$$2\Delta_1\Delta_2(A'-B') = 2\Delta_1^2\Delta_2 \tag{4.2.50}$$

from this

$$A'-B' = \Delta_1$$

Similarliy solving the linear equations ,eq(4.2.48) and eq(4.2.49)

$$A' = \frac{\Delta_1+\Delta_2}{2}$$

$$B' = \frac{\Delta_2-\Delta_1}{2}$$

$$\langle\langle C_{k-Q}\downarrow|C_k^\dagger\uparrow\rangle\rangle = \frac{1}{2}\left\{\frac{\Delta_1+\Delta_2}{(\omega^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2}+\frac{\Delta_2-\Delta_1}{(\omega^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2}\right\} \quad (4.2.51)$$

The superconducting order parameters (SCOP)can be related with Green's function as:

$$\Delta_1 = \frac{-V}{\beta}\sum_k \langle\langle C_{-k}^\dagger\downarrow|C_k^\dagger\uparrow\rangle\rangle \quad (4.2.52)$$

substituting eq(4.2.40) for$\langle\langle C_{-k}^\dagger\downarrow|C_k^\dagger\uparrow\rangle\rangle$,we will obtain the following:

$$\Delta_1 = \frac{-V}{2\beta}\sum_{k,n}\left\{\frac{\Delta_1+\Delta_2}{(\omega_n^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2}+\frac{\Delta_1-\Delta_2}{(\omega_n^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2}\right\} \quad (4.2.53)$$

where ω_n is the Matsubara frequency defined as

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

$$when, \omega_n \longmapsto i\omega_n$$

$$\Delta_1 = \frac{-V}{2\beta}\sum_{k,n}\left\{\frac{\Delta_1+\Delta_2}{(-(\frac{\pi(2n+1)}{\beta})^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2}+\frac{\Delta_1-\Delta_2}{(-(\frac{\pi(2n+1)}{\beta})^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2}\right\} \quad (4.2.54)$$

rearranging eq(4.2.54)

$$\Delta_1 = \frac{\beta V}{2}\sum_{k,n}\left\{\frac{\Delta_1+\Delta_2}{(\pi(2n+1)^2+\beta^2\{\epsilon_k^2+(\Delta_1+\Delta_2)^2\}}+\frac{\Delta_1-\Delta_2}{(\pi(2n+1))^2+\beta^2\{\epsilon_k^2+(\Delta_1-\Delta_2)^2\}}\right\} \quad (4.2.55)$$

Let N be the density of the state in momentum space which can be given by

$$N = \frac{1}{(2\pi)^3}\int\frac{d^3k}{e^{\beta(\epsilon_k-\mu)}+1} \quad (4.2.56)$$

OR

$$N(\epsilon) = \int_{-\epsilon_F}^{\infty} D(\epsilon)f(\epsilon)d\epsilon$$

where

$$f(\epsilon) = \frac{1}{e^{\beta(\epsilon_k-\mu)}+1}$$

this is Fermi-Dirac distribution which gives the probability that n orbital at energy ϵ will be occupied in an ideal electron gas in thermal equilibrium

$$\Delta_1 = \frac{\beta V}{2}\sum_n \int_{-\hbar\omega_F}^{\hbar\omega_F} D(\epsilon)\left\{\frac{\Delta_1+\Delta_2}{(\pi(2n+1)^2+\beta^2\{\epsilon_k^2+(\Delta_1+\Delta_2)^2\}}+\frac{\Delta_1-\Delta_2}{(\pi(2n+1))^2+\beta^2\{\epsilon_k^2+(\Delta_1-\Delta_2)^2\}}\right\} \tag{4.2.57}$$

$$\Delta_1 = \beta V N(0)\sum_n \int_0^{\hbar\omega_F} \left\{\frac{\Delta_1+\Delta_2}{(\pi(2n+1)^2+\beta^2\{\epsilon_k^2+(\Delta_1+\Delta_2)^2\}}+\frac{\Delta_1-\Delta_2}{(\pi(2n+1))^2+\beta^2\{\epsilon_k^2+(\Delta_1-\Delta_2)^2\}}\right\} \tag{4.2.58}$$

Let

$$\epsilon^2 = \epsilon_k^2 + (\Delta_1+\Delta_2)^2$$

$$\epsilon'^2 = \epsilon_k^2 + (\Delta_1-\Delta_2)^2$$

Define

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

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

$$\Delta_1 = \beta V N(0)\int_0^{\hbar\omega_F} \sum_n \left\{\frac{\Delta_1+\Delta_2}{(\pi(2n+1)^2+\beta^2\{\epsilon_k^2+(\Delta_1+\Delta_2)^2\}}+\frac{\Delta_1-\Delta_2}{(\pi(2n+1))^2+\beta^2\{\epsilon_k^2+(\Delta_1-\Delta_2)^2\}}\right\} \tag{4.2.59}$$

$$\Delta_1 = \beta V N(0)\int_0^{\hbar\omega_F} \left\{(\Delta_1+\Delta_2)\frac{\tanh\frac{\beta\epsilon}{2}}{2\beta\epsilon}+(\Delta_1-\Delta_2)\frac{\tanh\frac{\beta\epsilon'}{2}}{2\beta\epsilon'}\right\}d\epsilon \tag{4.2.60}$$

CASE 1

as T $\longmapsto$ T_c ,$\Delta_1 \longmapsto 0$

$$\frac{2}{\lambda} = \left[\int_0^{\hbar\omega_F}\left\{(1+\frac{\Delta_2}{\Delta_1})\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+(\Delta_1+\Delta_2)^2}}{2}}{\sqrt{\epsilon_k^2+(\Delta_1+\Delta_2)^2}}+(1-\frac{\Delta_2}{\Delta_1})\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}{2}}{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}\right\}d\epsilon\right], \tag{4.2.61}$$

Let I_1 and I_2 to be the integrals defined by

$$I_1 = \left[\int_0^{\hbar\omega_F}(1+\frac{\Delta_2}{\Delta_1})\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+(\Delta_1+\Delta_2)^2}}{2}}{\sqrt{\epsilon_k^2+(\Delta_1+\Delta_2)^2}}d\epsilon\right],$$

$$I_2 = \left[\int_0^{\hbar\omega_F}(1-\frac{\Delta_2}{\Delta_1})\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}{2}}{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}d\epsilon\right], \tag{4.2.62}$$

At the superconducting transition temperature the superconducting order parameter will become zero i.e

At $T = T_c$, $\Delta_1 = 0$.

then the first integral of I_1 can be written as

$$I_1' = \Big[\int_0^{\hbar\omega_F} \frac{\tanh \frac{\beta\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_2^2}} d\epsilon \Big], \tag{4.2.63}$$

eq(4.2.63) can be transformed by using the technique of Laplace transform and written as

$$I_1' = \Big[\int_0^{\hbar\omega_F} d\epsilon \frac{2}{\beta} \sum_{n=-\infty}^{n=\infty} \frac{1}{\omega_n^2+\epsilon^2} - \int_0^{\hbar\omega_F} \Delta_2^2 d\epsilon \frac{2}{\beta} \sum_{n=-\infty}^{n=\infty} \frac{1}{(\omega_n^2+\epsilon^2)^2} + ... \Big],$$

$$I_1' = \Big[\int_0^{\hbar\omega_F} \frac{\tanh \frac{\beta\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_2^2}} d\epsilon - \int_0^{\hbar\omega_F} \Delta_2^2 d\epsilon \frac{2}{\beta} \sum_{n=-\infty}^{n=\infty} \frac{1}{(\omega_n^2+\epsilon^2)^2} + ... \Big], \tag{4.2.64}$$

substituting the value for the Matsubara frequency

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

eq(4.2.64) can be rewritten as

$$I_1' = \Big[\int_0^{\hbar\omega_F} \frac{\tanh \frac{\beta\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_2^2}} d\epsilon - \int_0^{\hbar\omega_F} \Delta_2^2 d\epsilon \frac{2}{\beta} \sum_{n=-\infty}^{n=\infty} \frac{1}{(\frac{\pi(2n+1)}{\beta})^2+\epsilon^2)^2} + ... \Big],$$

rearranging this equation

$$I_1' = \Big[\int_0^{\hbar\omega_F} \frac{\tanh \frac{\beta\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_2^2}} d\epsilon - 2\beta^3\Delta_2^2 \int_0^{\hbar\omega_F} d\epsilon \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1))^4\{1+(\frac{\beta\epsilon}{\pi(2n+1)})^2\}^2} + ... \Big], \tag{4.2.65}$$

the first integral of eq(4.2.65) can be integrated by using integration by parts

Let

$$x = \frac{\beta\epsilon}{2}, dx = \frac{\beta d\epsilon}{2},$$

$$I_1'' = \int_0^{\frac{\beta\hbar\omega_F}{2}} \frac{\tanh x}{x} dx,$$

$$I_1'' = \left[\int_0^{\frac{\beta\hbar\omega_F}{2}} \frac{\tanh x}{x} dx \right], \tag{4.2.66}$$

$$\tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}}.$$

As $x \longmapsto \infty, then \tanh x \longmapsto 1.$

using this assumption eq(4.2.66) becomes

$$I_1'' = \left[\ln \frac{\beta\hbar\omega_F}{2} - \ln \frac{\pi}{4}(e^{-b}) = \ln 1.14\beta\hbar\omega_F \right], \tag{4.2.67}$$

where b is the Euler's constant and its value is b=0.577 which can be calculated from BCS relation i.e

$$\frac{2\Delta(0)}{T_c} \approx 2\pi e^{-b} \approx 3.50 where k_B = 1.$$

Let

$$I_1''' = \left[-2\beta^3\Delta_2^2 \int_0^{\hbar\omega_F} d\epsilon \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1))^4\{1 + (\frac{\beta\epsilon}{\pi(2n+1)})^2\}^2} + ... \right], \tag{4.2.68}$$

using substitution method we can integrate as

Let

$$y = \frac{\beta\epsilon}{\pi(2n+1)}, dy = \frac{\beta d\epsilon}{\pi(2n+1)},$$

then eq(4.2.68) can be rearranged as

$$I_1''' = \left[\frac{-4\Delta_2^2\beta^2}{\pi^3} \sum_{n=0}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^{\infty} \frac{1}{(1+y^2)^2} dy \right], \tag{4.2.69}$$

Define

$$\sum_{n=0}^{\infty} \frac{1}{(2n+1)^r} = (1 - 2^{-r})\zeta(r),$$

$$\oint_c f(z)dz = 2\pi i \sum Residue. \tag{4.2.70}$$

These are from the definitions of Riemann zeta functions and from the integration of functions having the singular points .we know the method of integration using Residue theorem .If f(z) has a pole of order m at z=a ,then

$$Res\{(f(z), a\} = \frac{1}{(m-1)!} \lim_{z \longrightarrow a} \frac{d^{m-1}}{dz^{m-1}}[(z-a)^m f(z)]$$

using this definition

$$\int_0^\infty \frac{1}{(1+y^2)^2} dy = \frac{\pi}{4}.$$

then eq(4.2.68) becomes

$$I_1''' = \left[\frac{-4\Delta_2^2\beta^2}{\pi^3} \sum_{n=0}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^\infty \frac{1}{(1+y^2)^2} dy \right] = \frac{-7\Delta_2^2\beta^2\zeta(3)}{8\pi^2}, \tag{4.2.71}$$

the second integral of I_1 is solved as follows

$$I_1'''' = \left[\int_0^{\hbar\omega_F} \lim_{\Delta_1 \longrightarrow 0} \left(\frac{\Delta_2}{\Delta_1} \frac{\tanh \frac{\beta\sqrt{\epsilon_k^2+(\Delta_1+\Delta_2)^2}}{2}}{\sqrt{\epsilon_k^2+(\Delta_1+\Delta_2)^2}} \right) d\epsilon \right], \tag{4.2.72}$$

this integral will have indeterminate form as the superconducting order parameter approaches 0 and it can be evaluated after differentiating both the numerators and denominators using L'Hopital's rule.

$$I_1'''' = \left[\int_0^{\hbar\omega_F} \lim_{\Delta_1 \longrightarrow 0} \left\{ \frac{\frac{\beta\Delta_2(\Delta_1+\Delta_2)\sec^2 \frac{\sqrt{\epsilon_k^2+(\Delta_1+\Delta_2)^2}}{2}}{2\sqrt{\epsilon_k^2+(\Delta_1+\Delta_2)^2}}}{\frac{\Delta_1(\Delta_1+\Delta_2)+1}{\sqrt{\epsilon_k^2+(\Delta_1+\Delta_2)^2}}} \right\} d\epsilon \right],$$

$$I_1'''' = \left[\int_0^{\hbar\omega_F} \frac{\beta\Delta_2^2 \sec^2 \beta\frac{\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{2(\epsilon_k^2+\Delta_2^2)} \right] \tag{4.2.73}$$

$$I_1'''' = \left[\int_0^{\hbar\omega_F} \left\{ \frac{\beta\Delta_2^2}{2(\epsilon_k^2+\Delta_2^2)} - \frac{\beta\Delta_2^2 \tanh^2 \beta\frac{\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{2(\epsilon_k^2+\Delta_2^2)} \right\} d\epsilon \right],$$

the first part of this integral can be evaluated using substitution method as

$$I_{1'}'''' = \left[\int_0^{\hbar\omega_F} \frac{\beta\Delta_2^2}{2(\epsilon_k^2+\Delta_2^2)} d\epsilon \right], \tag{4.2.74}$$

let

$$\epsilon_k = \Delta_2 \tan\gamma, then d\epsilon = \Delta_2\gamma \sec^2 d\gamma,$$

then

$$I_{1'}'''' = \left[\int_0^{\hbar\omega_F} \frac{\beta\Delta_2^2}{2(\epsilon_k^2+\Delta_2^2)} d\epsilon \right] = \left[\int_0^{\frac{\hbar\omega_F}{\Delta_2}} \frac{\beta\Delta_2}{2} d\gamma \right] = \left[\frac{\beta\Delta_2}{2} \arctan\frac{\hbar\omega_F}{\Delta_2} \right] = \left[\frac{\beta\Delta_2}{4} \ln\left\{ \frac{\hbar\omega_F+\Delta_2}{\hbar\omega_F-\Delta_2} \right\} \right]. \tag{4.2.75}$$

finally the total integral for I_1 is given by

$$I_1 = I_1''+I_1'''+I_1'''' = \Bigg[\ln 1.14\beta\hbar\omega_F - \frac{7\Delta_2^2\beta^2\zeta(3)}{8\pi^2} + \frac{\beta\Delta_2}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_2}{\hbar\omega_F-\Delta_2}\right\} - \int_0^{\hbar\omega_F}\left\{\frac{\beta\Delta_2^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{2(\epsilon_k^2+\Delta_2^2)}\right\}d\epsilon \tag{4.2.76}$$

$$I_2 = \Bigg[\int_0^{\hbar\omega_F}(1-\frac{\Delta_2}{\Delta_1})\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}{2}}{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}d\epsilon\Bigg], \tag{4.2.77}$$

$$I_2' = \Bigg[\int_0^{\hbar\omega_F}\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_2^2}}d\epsilon\Bigg], \tag{4.2.78}$$

$$I_2' = \Bigg[\int_0^{\hbar\omega_F}d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{\omega_n^2+\epsilon^2} - \int_0^{\hbar\omega_F}\Delta_2^2 d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{(\omega_n^2+\epsilon^2)^2} + ...\Bigg], \tag{4.2.79}$$

$$I_2' = \Bigg[\int_0^{\hbar\omega_F}\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_1^2}}d\epsilon - \int_0^{\hbar\omega_F}\Delta_2^2 d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{(\omega_n^2+\epsilon^2)^2} + ...\Bigg], \tag{4.2.80}$$

$$\omega_n = \frac{\pi(2n+1)}{\beta} \tag{4.2.81}$$

$$I_2'' = \Bigg[\int_0^{\hbar\omega_F}\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_2^2}}d\epsilon - \int_0^{\hbar\omega_F}\Delta_2^2 d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{(\frac{\pi(2n+1)}{\beta})^2+\epsilon^2)^2} + ...\Bigg], \tag{4.2.82}$$

$$x = \frac{\beta\epsilon}{2}, dx = \frac{\beta d\epsilon}{2}, \tag{4.2.83}$$

$$I_2'' = \Bigg[\int_0^{\frac{\beta\hbar\omega_F}{2}}\frac{\tanh x}{x}dx\Bigg], \tag{4.2.84}$$

$$\tanh x = \frac{e^x-e^{-x}}{e^x+e^{-x}}. \tag{4.2.85}$$

$$I_2'' = \ln\frac{\beta\hbar\omega_F}{2} - \ln(\frac{\pi}{4}(e^{-b}) = \ln 1.14\beta\hbar\omega_F, \tag{4.2.86}$$

where b is the Euler's constant and its value is b=0.577 which can be calculated from BCS relation i.e

$$\frac{2\Delta(0)}{T_c} \approx 2\pi e^{-b} \approx 3.50$$

where k_B=1.

$$I_2''' = \Big[-2\beta^3\Delta_2^2 \int_0^{\hbar\omega_F} d\epsilon \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1))^4\{1+(\frac{\beta\epsilon}{\pi(2n+1)})^2\}^2} + ...\Big], \tag{4.2.87}$$

using substitution method we can integrate as

Let

$$y = \frac{\beta\epsilon}{\pi(2n+1)}, dy = \frac{\beta d\epsilon}{\pi(2n+1)},$$

then eq(4.2.87) can be rearranged as

$$I_2''' = \Big[\frac{-4\Delta_2^2\beta^2}{\pi^3} \sum_{n=0}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^{\infty} \frac{1}{(1+y^2)^2} dy \Big], \tag{4.2.88}$$

using this definition

$$\int_0^{\infty} \frac{1}{(1+y^2)^2} dy = \frac{\pi}{4}.$$

$$I_2''' = \Big[\frac{-4\Delta_2^2\beta^2}{\pi^3} \sum_{n=0}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^{\infty} \frac{1}{(1+y^2)^2} dy \Big] = \Big[\frac{-7\Delta_2^2\beta^2\zeta(3)}{8\pi^2} \Big], \tag{4.2.89}$$

$$I_2'''' = \Big[\int_0^{\hbar\omega_F} \lim_{\Delta_1 \longrightarrow 0} \Big\{ \frac{\frac{\beta\Delta_2(\Delta_1-\Delta_2)\sec^2\frac{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}{2}}{2\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}}{\frac{\Delta_1(\Delta_1-\Delta_2)+1}{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}} \Big\} d\epsilon \Big], \tag{4.2.90}$$

$$I_2'''' = \Big[\int_0^{\hbar\omega_F} \frac{\beta\Delta_2^2 \sec^2 \beta\frac{\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{2(\epsilon_k^2+\Delta_2^2)} \Big], \tag{4.2.91}$$

$$I_2'''' = \Big[\int_0^{\hbar\omega_F} -\Big\{ \frac{\beta\Delta_2^2}{2(\epsilon_k^2+\Delta_2^2)} - \frac{\beta\Delta_2^2 \tanh^2 \beta\frac{\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{2(\epsilon_k^2+\Delta_2^2)} \Big\} d\epsilon \Big], \tag{4.2.92}$$

$$I_{2'}'''' = \Big[\int_0^{\hbar\omega_F} \frac{\beta\Delta_2^2}{2(\epsilon_k^2+\Delta_2^2)} d\epsilon \Big], \tag{4.2.93}$$

let

$$\epsilon_k = \Delta_2 \tan\gamma, then d\epsilon = \Delta_2\gamma \sec^2 d\gamma,$$

then

$$I_{2'}'''' = \Big[\int_0^{\hbar\omega_F} \frac{\beta\Delta_2^2}{2(\epsilon_k^2+\Delta_2^2)} d\epsilon \Big] = \Big[\int_0^{\frac{\hbar\omega_F}{\Delta_2}} \frac{\beta\Delta_2}{2} d\gamma \Big] = -\Big[-\frac{\beta\Delta_2}{2} \arctan\frac{\hbar\omega_F}{\Delta_2} \Big] = \Big[\frac{\beta\Delta_2}{4} \ln\Big\{ \frac{\hbar\omega_F+\Delta_2}{\hbar\omega_F-\Delta_2} \Big\} \Big]. \tag{4.2.94}$$

finally I_2 becocomes

$$I_2 = \left[\ln 1.14\beta\hbar\omega_F - \frac{7\Delta_2^2\beta^2\zeta(3)}{8\pi^2} + \frac{\beta\Delta_2}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_2}{\hbar\omega_F-\Delta_2}\right\} + \int_0^{\hbar\omega_F}\left\{\frac{\beta\Delta_2^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{2(\epsilon_k^2+\Delta_2^2)}\right\}d\epsilon\right]. \tag{4.2.95}$$

now eq(4.2.61)can be rewritten as the sumof I_1 and I_2.

$$\frac{2}{\lambda} = I_1 + I_2 = \ln 1.14\beta\hbar\omega_F - \frac{7\Delta_2^2\beta^2\zeta(3)}{8\pi^2} + \frac{\beta\Delta_2}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_2}{\hbar\omega_F-\Delta_2}\right\} - \int_0^{\hbar\omega_F}\left\{\frac{\beta\Delta_2^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{2(\epsilon_k^2+\Delta_2^2)}\right\}d\epsilon \tag{4.2.96}$$

$$+\ln 1.14\beta\hbar\omega_F - \frac{7\Delta_2^2\beta^2\zeta(3)}{8\pi^2} + \frac{\beta\Delta_2}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_2}{\hbar\omega_F-\Delta_2}\right\} + \int_0^{\hbar\omega_F}\left\{\frac{\beta\Delta_2^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{2(\epsilon_k^2+\Delta_2^2)}\right\}d\epsilon,$$

$$\frac{1}{\lambda} = \ln 1.14\beta\hbar\omega_F - \frac{7\Delta_2^2\beta^2\zeta(3)}{8\pi^2} - \frac{\beta\Delta_2}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_2}{\hbar\omega_F-\Delta_2}\right\}. \tag{4.2.97}$$

Let

$$b = \frac{\beta}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_2}{\hbar\omega_F-\Delta_2}\right\},$$

and neglecting the second (higher order) and the Fourth terms from eq(4.2.97)

rearranging this expression the superconducting transition temperature can be given by the relation

$$T_c = \frac{1.14\hbar\omega_F}{k_B}e^{-\{\frac{1}{\lambda}+b\Delta_2\}}. \tag{4.2.98}$$

CASE 2

The superconducting order parameter of spin density wave can be related with Green's function as

$$\Delta_2 = -\frac{U}{\beta}\sum_k \langle\langle C_{k-Q}\downarrow | C_k^\dagger\uparrow\rangle\rangle = -\frac{U}{2\beta}\sum_k\left\{\frac{\Delta_1+\Delta_2}{(\omega^2-\epsilon_k^2)-(\Delta_1+\Delta_2)^2} + \frac{\Delta_2-\Delta_1}{(\omega^2-\epsilon_k^2)-(\Delta_1-\Delta_2)^2}\right\}, \tag{4.2.99}$$

using the same procedure that we have used to calculate the transition temperature in case 1 here we can also determine the spin density wave transition temperature

$$\Delta_2 = \left[\frac{U}{2\beta}\sum_{k,n}\left\{\frac{\Delta_1+\Delta_2}{((\frac{\pi(2n+1)}{\beta})^2+\epsilon_k^2)+(\Delta_1+\Delta_2)^2} + \frac{\Delta_2-\Delta_1}{((\frac{\pi(2n+1)}{\beta})^2+\epsilon_k^2)+(\Delta_1-\Delta_2)^2}\right\}\right], \tag{4.2.100}$$

This equation can be also expressed using definition of hyperbolic function given in eq(4.2.60)

$$\Delta_2 = \left[\frac{\beta^2 U}{2\beta}\sum_k \left\{(\Delta_1+\Delta_2)\frac{\tanh\frac{\beta\epsilon}{2}}{2\beta\epsilon} + (\Delta_2-\Delta_1)\frac{\tanh\frac{\beta\epsilon'}{2}}{2\beta\epsilon'}\right\}\right], \tag{4.2.101}$$

$$\Delta_2 = \left[\frac{U}{2}\int_0^{\hbar\omega_F} D(\epsilon)\left\{(\Delta_1+\Delta_2)\frac{\tanh\frac{\beta\epsilon}{2}}{\epsilon} + (\Delta_2-\Delta_1)\frac{\tanh\frac{\beta\epsilon'}{2}}{\epsilon'}\right\}d\epsilon\right], \tag{4.2.102}$$

$$= \left[\frac{N(0)U}{2}\int_0^{\hbar\omega_F} \left\{(\Delta_1+\Delta_2)\frac{\tanh\frac{\beta\epsilon}{2}}{\epsilon} + (\Delta_2-\Delta_1)\frac{\tanh\frac{\beta\epsilon'}{2}}{\epsilon'}\right\}d\epsilon\right],$$

define N(0)U=λ'

$$\frac{2}{\lambda'} = \left[\int_0^{\hbar\omega_F} \left\{(1+\frac{\Delta_1}{\Delta_2})\frac{\tanh\frac{\beta\epsilon}{2}}{\epsilon} + (1-\frac{\Delta_1}{\Delta_2})\frac{\tanh\frac{\beta\epsilon'}{2}}{\epsilon'}\right\}d\epsilon\right] \tag{4.2.103}$$

In SDW region as $T \longmapsto T_{sdw}, \Delta_{sdw} = \Delta_2 \longmapsto 0$.

Let J_1 and J_2 integrals defined by

$$J_1 = \left[\int_0^{\hbar\omega_F} (1+\frac{\Delta_1}{\Delta_2})\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}{2}}{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}d\epsilon\right],$$

$$J_2 = \left[\int_0^{\hbar\omega_F} (1-\frac{\Delta_1}{\Delta_2})\frac{\tanh\frac{\beta\sqrt{(\epsilon_k^2+(\Delta_1-\Delta_2)^2}}{2}}{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}d\epsilon\right],$$

using the same procedure used before the first integral of J_1 can be transformed using Laplace transform as

$$J_1' = \left[\int_0^{\hbar\omega_F} d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{\omega_n^2+\epsilon^2} - \int_0^{\hbar\omega_F}\Delta_1^2 d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{(\omega_n^2+\epsilon^2)^2} + ...\right], \tag{4.2.104}$$

substituting the value for the Matsubara frequency eq(4.2.104) will be

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

$$J_1' = \Bigg[\int_0^{\hbar\omega_F} \frac{\tanh \frac{\beta\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_1^2}} d\epsilon - \int_0^{\hbar\omega_F} \Delta_1^2 d\epsilon \frac{2}{\beta} \sum_{n=-\infty}^{n=\infty} \frac{1}{(\frac{\pi(2n+1)}{\beta})^2+\epsilon^2)^2} + ... \Bigg], \quad (4.2.105)$$

the first integral of eq(4.2.105) can be integrated by using integration by parts i.e

$$J_1'' = \Bigg[\int_0^{\hbar\omega_F} \frac{\tanh \frac{\beta\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_1^2}} d\epsilon \Bigg], \quad (4.2.106)$$

Let

$$x = \frac{\beta\epsilon}{2}, dx = \frac{\beta d\epsilon}{2},$$

$$J_1'' = \Bigg[\int_0^{\frac{\beta\hbar\omega_F}{2}} \frac{\tanh x}{x} dx \Bigg] = \Bigg[\ln \frac{\beta\hbar\omega_F}{2} - \ln \frac{\pi}{4}(e^{-b}) \Bigg] = \ln 1.14\beta\hbar\omega_F,$$

similarly the second integral of J_1'can be integrated as

$$J_1''' = \Bigg[-2\beta^3\Delta_1^2 \int_0^{\hbar\omega_F} d\epsilon \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1))^4\{1+(\frac{\beta\epsilon}{\pi(2n+1)})^2\}^2} + ... \Bigg], \quad (4.2.107)$$

using substitution method we can integrate as

Let

$$y = \frac{\beta\epsilon}{\pi(2n+1)}, dy = \frac{\beta d\epsilon}{\pi(2n+1)},$$

then eq(4.2.107) can be rearranged as

$$J_1''' = \Bigg[\frac{-4\Delta_1^2\beta^2}{\pi^3} \sum_{n=0}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^{\infty} \frac{1}{(1+y^2)^2} dy \Bigg], \quad (4.2.108)$$

using the definition

$$\int_0^{\infty} \frac{1}{(1+y^2)^2} dy = \frac{\pi}{4}.$$

$$J_1''' = \Bigg[\frac{-4\Delta_1^2\beta^2}{\pi^3} \sum_{n=0}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^{\infty} \frac{1}{(1+y^2)^2} dy \Bigg] = \frac{-7\Delta_1^2\beta^2\zeta(3)}{8\pi^2}, \quad (4.2.109)$$

the second integral of J_1 has indetrminate form as $\Delta_2$apporoaches 0 ,therefore we should differentiate both numerator and denominator using L'Hopitals rule

$$J_1'''' = \left[\int_0^{\hbar\omega_F} \lim_{\Delta_2 \longrightarrow 0} \left\{ \frac{\frac{\beta\Delta_1(\Delta_1-\Delta_2)\sec^2\frac{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}{2}}{2\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}}{\frac{\Delta_2(\Delta_1-\Delta_2)+1}{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}} \right\} d\epsilon \right], \tag{4.2.110}$$

$$J_1'''' = \left[\int_0^{\hbar\omega_F} \left\{ \frac{\beta\Delta_1^2}{2(\epsilon_k^2+\Delta_1^2)} - \frac{\beta\Delta_1^2 \tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{2(\epsilon_k^2+\Delta_1^2)} \right\} d\epsilon \right], \tag{4.2.111}$$

the first part of this integral can evaluated using substitution method as

$$J_{1'}'''' = \left[\int_0^{\hbar\omega_F} \frac{\beta\Delta_1^2}{2(\epsilon_k^2+\Delta_1^2)} d\epsilon \right], \tag{4.2.112}$$

let

$$\epsilon_k = \Delta_1 \tan\gamma, then d\epsilon = \Delta_1\gamma\sec^2\gamma d\gamma,$$

then

$$J_{1'}'''' = \left[\int_0^{\hbar\omega_F} \frac{\beta\Delta_1^2}{2(\epsilon_k^2+\Delta_1^2)} d\epsilon \right] = \left[\int_0^{\frac{\hbar\omega_F}{\Delta_1}} \frac{\beta\Delta_1}{2} d\gamma \right] = \left[\frac{\beta\Delta_1}{2}\arctan\frac{\hbar\omega_F}{\Delta_1}\right] = \left[\frac{\beta\Delta_1}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_1}{\hbar\omega_F-\Delta_1}\right\}\right]. \tag{4.2.113}$$

Finally we will obtain J_1.

$$J_1 = \ln 1.14\beta\hbar\omega_F - \frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2} + \frac{\beta\Delta_1}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_1}{\hbar\omega_F-\Delta_1}\right\} - \int_0^{\hbar\omega_F} \frac{\beta\Delta_1^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{2(\epsilon_k^2+\Delta_1^2)} d\epsilon. \tag{4.2.114}$$

the second integral parts of SDW can also integrated using the same approach

$$J_2 = \left[\int_0^{\hbar\omega_F} (1-\frac{\Delta_1}{\Delta_2}) \frac{\tanh\frac{\beta\sqrt{(\epsilon_k^2+(\Delta_1-\Delta_2)^2}}{2}}{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}} d\epsilon \right], \tag{4.2.115}$$

the first part of J_2 can be transformed using Laplace transform

$$J'2 = \left[\int_0^{\hbar\omega_F} d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{\omega_n^2+\epsilon^2} - \int_0^{\hbar\omega_F}\Delta_1^2 d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{(\omega_n^2+\epsilon^2)^2} + ...\right], \tag{4.2.116}$$

substituting the value for the Matsubara frequency eq(4.2.116) will be

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

$$J_2' = \Bigg[\int_0^{\hbar\omega_F} \frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_1^2}} d\epsilon - \int_0^{\hbar\omega_F} \Delta_1^2 d\epsilon \frac{2}{\beta} \sum_{n=-\infty}^{n=\infty} \frac{1}{(\frac{\pi(2n+1)}{\beta})^2+\epsilon^2)^2} + ... \Bigg], \quad (4.2.117)$$

the first integral of eq(4.2.117) can be integrated by using integration by parts i.e

$$J_2'' = \Bigg[\int_0^{\hbar\omega_F} \frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_1^2}} d\epsilon \Bigg], \quad (4.2.118)$$

Let

$$x = \frac{\beta\epsilon}{2}, dx = \frac{\beta d\epsilon}{2},$$

$$J_2'' = \int_0^{\frac{\beta\hbar\omega_F}{2}} \frac{\tanh x}{x} dx = \left[\ln\frac{\beta\hbar\omega_F}{2} - \ln\frac{\pi}{4}(e^{-b}) \right] = \ln 1.14\beta\hbar\omega_F,$$

Similarly the second integral of eq(4.2.117)

$$J_2''' = \Bigg[-2\beta^3\Delta_1^2 \int_0^{\hbar\omega_F} d\epsilon \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1))^4\{1+(\frac{\beta\epsilon}{\pi(2n+1)})^2\}^2} + ... \Bigg], \quad (4.2.119)$$

using substitution method we can integrate as

Let

$$y = \frac{\beta\epsilon}{\pi(2n+1)}, dy = \frac{\beta d\epsilon}{\pi(2n+1)},$$

then eq(4.2.119) can be rearranged as

$$J_2''' = \Bigg[\frac{-4\Delta_1^2\beta^2}{\pi^3} \sum_{n=0}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^{\infty} \frac{1}{(1+y^2)^2} dy \Bigg], \quad (4.2.120)$$

using the definition

$$\int_0^{\infty} \frac{1}{(1+y^2)^2} dy = \frac{\pi}{4}.$$

$$J_2''' = \left[\frac{-4\Delta_1^2\beta^2}{\pi^3}\sum_{n=0}^{n=\infty}\frac{1}{(2n+1)^3}\int_0^\infty \frac{1}{(1+y^2)^2}dy\right] = -\frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2}, \tag{4.2.121}$$

the second integral of J_2 has indeterminate form as Δ_2 apporoaches 0 , therefore we should differentiate both numerator and denominator using L'Hopitals rule.

$$J_2'''' = \left[\int_0^{\hbar\omega_F} \lim_{\Delta_2\longrightarrow 0}\left\{\frac{\frac{\beta\Delta_1(\Delta_1-\Delta_2)\sec^2\frac{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}{2}}{2\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}}{\frac{\Delta_2(\Delta_1-\Delta_2)+1}{\sqrt{\epsilon_k^2+(\Delta_1-\Delta_2)^2}}}\right\}d\epsilon\right], \tag{4.2.122}$$

$$J_2'''' = \left[\int_0^{\hbar\omega_F}\left\{\frac{\beta\Delta_1^2}{2(\epsilon_k^2+\Delta_1^2)} - \frac{\beta\Delta_1^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{2(\epsilon_k^2+\Delta_1^2)}\right\}d\epsilon\right], \tag{4.2.123}$$

$$J_2'''' = \left[\int_0^{\hbar\omega_F}\left\{\frac{\beta\Delta_1^2}{2(\epsilon_k^2+\Delta_1^2)} - \frac{\beta\Delta_1^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{2(\epsilon_k^2+\Delta_1^2)}\right\}d\epsilon\right],$$

the first part of this integral can evaluated using substitution method as

$$J_{2'}'''' = \int_0^{\hbar\omega_F}\frac{(\beta\Delta_1^2)}{2(\epsilon_k^2+\Delta_1^2)}d\epsilon, \tag{4.2.124}$$

let

$$\epsilon_k = \Delta_1\tan\gamma, then d\epsilon = \Delta_1\gamma\sec^2\gamma d\gamma,$$

then

$$J_{2'}'''' = \int_0^{\hbar\omega_F}(\frac{\beta\Delta_1^2}{2(\epsilon_k^2+\Delta_1^2)})d\epsilon = \int_0^{\frac{\hbar\omega_F}{\Delta_1}}\frac{\beta\Delta_1}{2}d\gamma = \frac{\beta\Delta_1}{2}\arctan\frac{\hbar\omega_F}{\Delta_1}, \tag{4.2.125}$$
$$= \frac{\beta\Delta_1}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_1}{\hbar\omega_F-\Delta_1}\right\},$$

then the final integral for J_2 will be

$$J_2 = \ln 1.14\beta\hbar\omega_F - \frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2} + \frac{\beta\Delta_1}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_1}{\hbar\omega_F-\Delta_1}\right\} - \int_0^{\hbar\omega_F}\frac{\beta\Delta_1^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{2(\epsilon_k^2+\Delta_1^2)}d\epsilon. \tag{4.2.126}$$

Finally eq(4.2.103) can be rewritten as

$$\frac{2}{\lambda'} = \ln 1.14\beta\hbar\omega_F - \frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2} + \frac{\beta\Delta_1}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_1}{\hbar\omega_F-\Delta_1}\right\} - \int_0^{\hbar\omega_F}\frac{\beta\Delta_1^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{2(\epsilon_k^2+\Delta_1^2)}d\epsilon \tag{4.2.127}$$

$$+\ln 1.14\beta\hbar\omega_F + \frac{-7\Delta_1^2\beta^2\zeta(3)}{8\pi^2} + \frac{\beta\Delta_1}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_1}{\hbar\omega_F-\Delta_1}\right\} - \int_0^{\hbar\omega_F}\frac{\beta\Delta_1^2\tanh^2\beta\frac{\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{2(\epsilon_k^2+\Delta_1^2)}d\epsilon.$$

$$\frac{1}{\lambda'} = \ln 1.14\beta\hbar\omega_F - \frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2} + \frac{\beta\Delta_1}{4}\ln\left\{\frac{\hbar\omega_F+\Delta_1}{\hbar\omega_F-\Delta_1}\right\}$$

Similarly neglecting the higher order (second term) and Fourth term from eq(4.2.127),

Finally the spin density wave transition temperature can be determined from the above equations as

$$T_{sdw} = T_2 = \frac{1.14\hbar\omega_F}{k_B}e^{-\{\frac{1}{\lambda'}-b\Delta_1\}}. \tag{4.2.128}$$

4.2.1 Superconducting Order parameter in pure superconducting region

In pure superconducting region the superconducting order parmeter of the spin density wave will become zero i.e $\Delta_2 \longrightarrow 0$.

$$\frac{1}{\lambda} = \left[\int_0^{\hbar\omega_F}\left\{\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_1^2}}\right\}d\epsilon\right], \tag{4.2.129}$$

eq(4.2.129) can be transformed by using the technique of Laplace transform and written as

$$I_1' = \left[\int_0^{\hbar\omega_F} d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{\omega_n^2+\epsilon^2} - \int_0^{\hbar\omega_F}\Delta_1^2 d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{(\omega_n^2+\epsilon^2)^2} + ...\right], \tag{4.2.130}$$

substituting the value for the Matsubara frequency

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

$$I_1' = \left[\int_0^{\hbar\omega_F}\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+\Delta_1^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_1^2}}d\epsilon - \int_0^{\hbar\omega_F}\Delta_1^2 d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{(\frac{\pi(2n+1)}{\beta})^2+\epsilon^2)^2} + ...\right], \tag{4.2.131}$$

the first integral of eq(4.2.131) can be integrated by using integration by parts.

Let

$$x = \frac{\beta\epsilon}{2}, dx = \frac{\beta d\epsilon}{2},$$

$$I_1'' = \int_0^{\frac{\beta\hbar\omega_F}{2}} \frac{\tanh x}{x} dx,$$

$$I_1'' = \left[\int_0^{\frac{\beta\hbar\omega_F}{2}} \frac{\tanh x}{x} dx \right], \tag{4.2.132}$$

As $x \longmapsto \infty, then \tanh x \longmapsto 1$.

using this assumption eq(4.2.132) becomes

$$I_1'' = \left[\ln \frac{\beta\hbar\omega_F}{2} - \ln \frac{\pi}{4}(e^{-b}) \right] = \ln 1.14\beta\hbar\omega_F,$$

Let

$$I_1''' = \left[-2\beta^3\Delta_1^2 \int_0^{\hbar\omega_F} d\epsilon \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1))^4\{1+(\frac{\beta\epsilon}{\pi(2n+1)})^2\}^2} + ... \right], \tag{4.2.133}$$

using substitution method we can integrate as

Let

$$y = \frac{\beta\epsilon}{\pi(2n+1)}, dy = \frac{\beta d\epsilon}{\pi(2n+1)},$$

then eq(4.2.133) can be rearranged as

$$I_1''' = \left[\frac{-4\Delta_1^2\beta^2}{\pi^3} \sum_{n=0}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^{\infty} \frac{1}{(1+y^2)^2} dy \right] = -\frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2}, \tag{4.2.134}$$

Finally eq(4.2.129) can be written as

$$\frac{1}{\lambda} = \ln 1.14\beta\hbar\omega_F - \frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2}, \tag{4.2.135}$$

In pure superconducting region eq(4.2.98) can be reduced in to BCS expression as

$$T_c = 1.14\frac{\hbar\omega_F}{k_B} e^{-\frac{1}{\lambda}}. \tag{4.2.136}$$

From this we can get the following relation

$$\frac{1}{\lambda} = \ln 1.14\frac{\hbar\omega_F}{k_B T_c}, \tag{4.2.137}$$

Equating eq(4.2.135) and eq(4.2.137) we will get

$$\ln 1.14\frac{\hbar\omega_F}{k_B T_c} = \ln 1.14\frac{\hbar\omega_F}{k_B T} - \frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2}, \tag{4.2.138}$$

rearranging eq(4.2.138) we can have

$$\ln(\frac{T}{T_c}) = -\frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2}, \tag{4.2.139}$$

This can be rewritten as

$$\ln(1-(1-(\frac{T}{T_c}))) = -\frac{7\Delta_1^2\beta^2\zeta(3)}{8\pi^2}, \tag{4.2.140}$$

But

$$\ln(1-(1-y)) = -(1-y) - \frac{(1-y)^2}{2} + ...,$$

using this ,eq(4.2.140) will be given by the relation

$$k_B^2T_c^2(1-(\frac{T}{T_c})) \approx \frac{7\Delta_1^2\zeta(3)}{8\pi^2}, \tag{4.2.141}$$

then

$$\Delta_1(T) = 3.06k_BT_c\sqrt{1-(\frac{T}{T_c})}. \tag{4.2.142}$$

4.2.2 Spin density wave order parameter in pure spin density wave region

In pure spin density wave region the superconducting order parameter will become zero i.e $\Delta_1 \longrightarrow 0$.

$$\frac{1}{\lambda'} = \Big[\int_0^{\hbar\omega_F}\Big\{\frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_2^2}}\Big\}d\epsilon\Big], \tag{4.2.143}$$

eq(4.2.143) can be transformed by using the technique of Laplace transform and written as

$$J_1' = \Big[\int_0^{\hbar\omega_F} d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{\omega_n^2+\epsilon^2} - \int_0^{\hbar\omega_F}\Delta_2^2 d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{(\omega_n^2+\epsilon^2)^2} + ...\Big], \tag{4.2.144}$$

$$J_1' = \Big[\int_0^{\hbar\omega_F} d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{\omega_n^2+\epsilon^2} - \int_0^{\hbar\omega_F}\Delta_2^2 d\epsilon\frac{2}{\beta}\sum_{n=-\infty}^{n=\infty}\frac{1}{(\omega_n^2+\epsilon^2)^2} + ...\Big], \tag{4.2.145}$$

substituting the value for the Matsubara frequency

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

$$J_1' = \Bigg[\int_0^{\hbar\omega_F} \frac{\tanh\frac{\beta\sqrt{\epsilon_k^2+\Delta_2^2}}{2}}{\sqrt{\epsilon_k^2+\Delta_2^2}} d\epsilon - \int_0^{\hbar\omega_F} \Delta_2^2 d\epsilon \frac{2}{\beta} \sum_{n=-\infty}^{n=\infty} \frac{1}{(\frac{\pi(2n+1)}{\beta})^2+\epsilon^2)^2} + ... \Bigg], \quad (4.2.146)$$

the first integral of eq(4.2.146) can be integrated by using integration by parts and finally eq(4.2.143) will become

$$\frac{1}{\lambda'} = \ln 1.14 \frac{\hbar\omega_F}{k_B T} - \frac{7\Delta_2^2\beta^2\zeta(3)}{8\pi^2}, \quad (4.2.147)$$

But from eq(4.2.128)

$$T_{sdw} = T_2 = \frac{1.14\hbar\omega_F}{k_B} e^{-\{\frac{1}{\lambda'} - b\Delta_1\}}.$$

rearranging this

$$\frac{1}{\lambda'} = \ln 1.14 \frac{\hbar\omega_F}{k_B T_{sdw}}, \quad (4.2.148)$$

Equating eq(4.2.147) and eq(4.2.148) we will get

$$\ln 1.14 \frac{\hbar\omega_F}{k_B T_{sdw}} = \ln 1.14 \frac{\hbar\omega_F}{k_B T} - \frac{7\Delta_2^2\beta^2\zeta(3)}{8\pi^2}, \quad (4.2.149)$$

This can be rewritten as

$$\ln(1-(1-(\frac{T}{T_{sdw}})) = -\frac{7\Delta_2^2\beta^2\zeta(3)}{8\pi^2}, \quad (4.2.150)$$

$$k_B^2 T_{sdw}^2 (1-(\frac{T}{T_{sdw}})) \approx \frac{7\Delta_2^2\zeta(3)}{8\pi^2}, \quad (4.2.151)$$

$$\Delta_2(T) = 3.06 k_B T_{sdw} \sqrt{1-(\frac{T}{T_{sdw}})}. \quad (4.2.152)$$

Chapter 5

Results and Discussions

In this paper we have used the Model Hamiltonian which can be described in quantized form using annihilation and creation operators of the given system.Green's function formalism helped to write equation of motion,using this formalism we have found eq(4.2.53) and eq(4.2.100) that relates the superconducting and spin density wave order parameters which helped us to determine the transition temperature for SC and SDW. Using the equation of motion we have found the exponential function the connects the order parameters with transition temperature.Based on the function again we ploted the graph to show the coexistence between superconductivity and spin density wave.Moreover, the effect of spin density wave on superconductivity is clearly shown on this theoretical work.Spin density wave of ferropnictides(122)families is due to delocalized d-orbital electron.When we consider special case i.e spin density wave order parameter($\Delta_2 \longrightarrow 0$),then we have got pure superconducting region and finally reduced to BCS expression.From eq(4.2.98) we observed that the spin density wave order parameter supresses the transition temperature of superconductiviy.

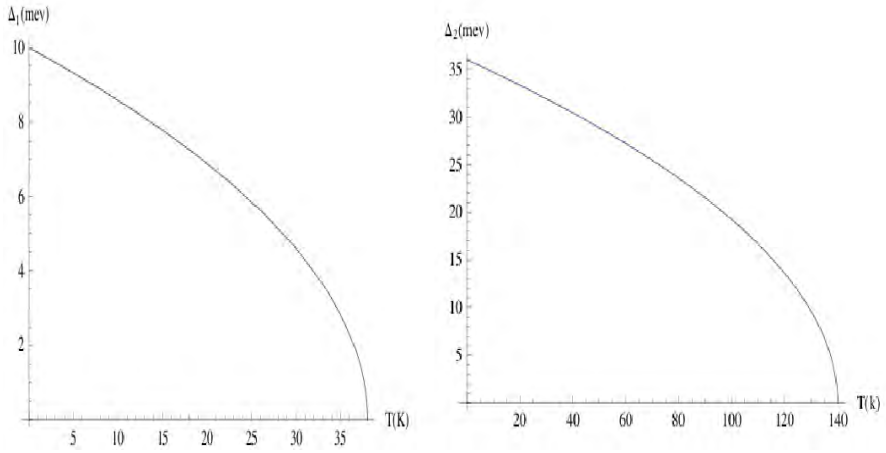

Figure 5.1: Superconducting order parameter vs temperature

Figure 5.2: Spin density wave order parameter vs temperature

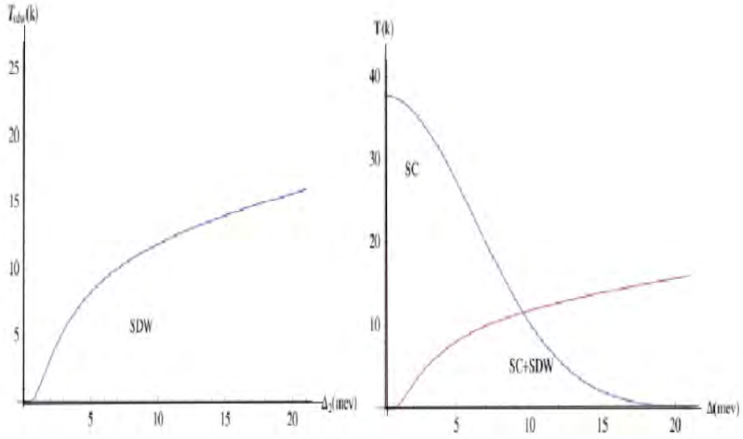

Figure 5.3: Spin density wave ordering temperature vs spin density wave order parameter

Figure 5.4: Temperature of coexistence of superconductivity and spin density wave vs order parameter

Chapter 6

Conclusion

In this thesis the historical discovery of superconductivity such as low dimensional organic superconductors ,cuprate superconductors and recently discovered iron based superconductors have been discussed.The first evidence of interplay between spin density wave and superconductivity in ferropnictides particularly $Ba_{1-x}K_xFe_2As_2$ was the presence of anti-ferromagnetic ordering in some region.The coexistence of superconductivity and spin density wave has been discussed using the Model Hamiltonian which can be expressed using operators(anni-hilation and creation) .We have used the Green's function formalism to find the equation of motion that help us to determine the superconducting and spin density wave order parameters.The magnetic ordering,concentration dependent phase diagram for $Ba_{1-x}K_xFe_2As_2$ which shows the coexistence of superconductivity and spin density wave is possible in $Ba_{1-x}K_xFe_2As_2$ which is in a good agreement with experimental observation.

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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: Sewnet Demelash Yihun

Signature:– – – – – – – – – – – –

Place and time of submission: Addis Ababa University, June 2011

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

Name: Prof. singh

Signature:– – – – – – – – – ––