THE STUDY OF COEXISTENCE OF SUPERCONDUCTIVITY AND SPIN DENSITY WAVE (SDW) IN $SmO_{1-x}F_xFeAs$

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By

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The undersigned hereby certify that they have read and recommended to the Faculty of Science School of Graduate Studies for acceptance a thesis entitled “THE STUDY OF CO-EXISTENCE OF SUPERCONDUCTIVITY AND SPIN DENSITY WAVE (SDW) IN $SmO_{1-x}F_xFeAs$” by Dagne Atnafu Master of Science in partial fulfillment of the requirements for the degree of Master of Science in Physics.

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This work is dedicated to my family

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Abstract

Superconductivity and magnetism were previously thought as incompatible until the discovery of some rare earth ternary compounds that shows the coexistence of superconductivity and magnetism. In some of the recently discovered iron-based layered superconductors superconductivity and magnetism are coexist. In the present work we examine the possibility of coexistence of superconductivity and spin density wave in samarium arsenide oxide superconductor ($SmO_{1-x}F_xFeAs$). Using the model of the Hamiltonian and retarded double time green's function formalism, we found mathematical expression for superconducting transition temperature (T_c), superconductivity order parameter (Δ_{sc}), spin density wave order parameter (M), and spin density wave transition temperature (T_{sdw}). We merged the phase diagram of T_c vs. M and T_{sdw} vs. M, to obtain the region where both orders i.e. superconductivity and spin density wave coexist. The region under the intersection of the two merged graphs shows that superconductivity and spin density wave coexist in the system.

Introduction

Superconductivity is a phenomenon occurring in a certain materials at extremely low temperature, characterized by exactly zero electrical resistance. It was discovered in 1911 by Heike kamerlingh Onnes, who was studying the resistance of solid mercury at extremely low temperatures using the recently-discovered liquid helium as a refrigerant. At the temperature about 4.2K, he observed that the resistance abruptly disappeared [1]. Superconductivity has been found early in various elements such as mercury, lead, and aluminum. Most of the early superconductors are superconducting at extremely low transition temperature and low magnetic field.

Until 1986 the record for highest critical temperature was 23K for Nb_3Ge. In 1986 a new La-Ba-based copper-oxide superconductor, (La, Ba) $_2CuO_4$, with critical temperature of 35K was discovered by Alex Müller and Georg Bednorz [2]. During the past decades it was subsequently established that superconductivity in all of these “high temperature” superconductors (HTS) containing Y, Bi, Tl, and Hg instead of La can be maintained up to much higher magnetic field and temperature. Moreover, materials of this class of oxides have been discovered with transition temperature well above 100K. In 2001, the discovery of non-oxide based superconductor in MgB_2 by Nagamatsu and Akimitsu [3] has restored the huge interest in the field of superconductivity.

In February 2008, Hideo Hoson(from the Tokyo Institute of Technology in Japan) [4] has discovered an iron-based superconducting material in LaOFFeAs. The critical temperature for this iron-arsenide compound with lanthanum, oxygen and fluorine is 26K. Moreover, subsequent studies clarified that replacement of La by other rare earth elements increases the transition temperature markedly: 41K for Ce, 52K for Pr, 52K for Nd, and 55K for Sm. Superconductivity has also been discovered in fluorine-free systems, including $RFeAsO_{1-y}$

(R=La, Ce, Pr, Nd, Sm, Gd and T_c = 31K-55K), it was surprising that there could be another material other than the cuprate which could become superconducting at such elevated temperatures. The recent discovery of non-oxide superconductors in MgB_2 and iron-based compound ROFFeAs would also assist theoretical physicists to be closer to a fundamental understanding in the basic mechanism behind high-temperature superconductivity.

Most of the physical properties of superconductors vary from material to material, such as the heat capacity, the critical temperature, critical current density, and critical field at which superconductivity is destroyed. However, there is a class of properties that are not dependent of the mentioned material. For instance, all superconductors have exactly zero resistance.

The interplay between superconductivity and magnetism has been an interesting topic in condensed mater physics. Superconductivity and magnetism are often thought to be incompatible. According to BCS theory of superconductivity, a superconductor expels a magnetic field, which in turn destroys superconductivity. However, both superconductivity and magnetic ordering has been seen in harmony (coexists) in some of rare earth compound. The coexistence of superconductivity and antiferromagnetism is quite peaceful and very weakly influences each other. The recent discovery of superconductivity in the rare-earth iron-based oxide system ($RO_{1-x}F_xFeAs$), it is generally believed that magnetism play fundamental role in superconducting mechanism like copper-oxide because superconductivity occurs when mobile electrons or holes are doped into SDW parent compound. Experiment has been revealed that superconducting and magnetic phases coexist in samarium iron pnictide superconductor ($SmFeAs(O_{1-x}F_x)$) with the long range of ($0.1 \leq x \leq 0.13$).

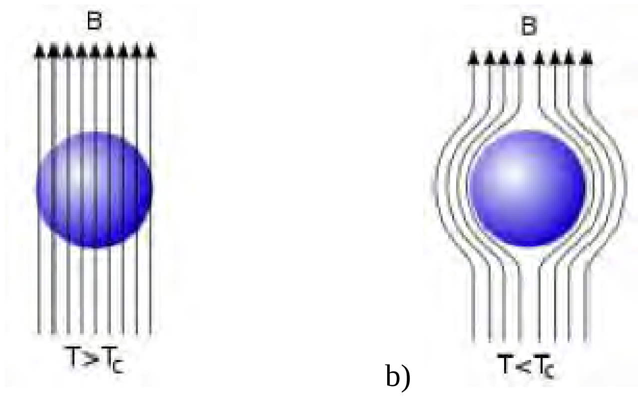
In this paper we studied theoretical coexistence of superconductivity and spin density wave (SDW) in $SmFeAs(O_{1-x}F_x)$. For this reason we include literature review on magnetism, superconductivity, and iron based superconductors in the first chapter, mathematical method in the second chapter, and the third on formulation of the problem, in the fourth chapter we include results and discussion and in the final chapter we put some important conclusions of the study.

Chapter 1

Literature Review

1.1 Meissner effect

The Meissner effect was discovered in 1933 by Water Meissner and Robert Ochsnfield [5]. It is one of the properties of superconducting materials. When a superconductor below T_c is placed under a weak external magnetic field B, it repels the magnetic flux (field) B completely from its interior. It does this by setting up electric currents near its surface. It is the magnetic field of these surface currents that cancels out the applied magnetic field within the bulk of the superconductor. However, near the surface, within a distance called the London penetration depth, the magnetic field is not completely cancelled; this region also contains the electric currents whose field cancels the applied magnetic field within the bulk. This exclusion of magnetic flux from superconductor (B=0) is known as Meissner effect.



a) b)

Fig.1.1. The Meissner effect a) Magnetic field penetrating a superconductor above critical temperature
b) Magnetic field expelled from it below the critical temperature

Source: http://en.wikipedia.org/wiki/Meissner_effect

1.2 Types of superconductors

Superconductors can be type I and type II according to their behavior in a magnetic field [6]. In type I, superconductivity is abruptly destroyed when the strength of the applied field rises above the critical value. Most pure elemental superconductors, except niobium, technetium, and vanadium are type I. In type II superconductors, raising the applied field beyond a critical value B_{c1} lead to a mixed state in which increasing amount of magnetic flux penetrates the material, but there remains no resistance to the flow of electrical current. At the second critical field B_{c2}, superconductivity is destroyed. Type II superconductors show two critical magnetic field values, one at the onset of a mixed superconducting and the normal state and one where superconducting ceases. Almost all impure and compound superconductors are Type II superconductors.

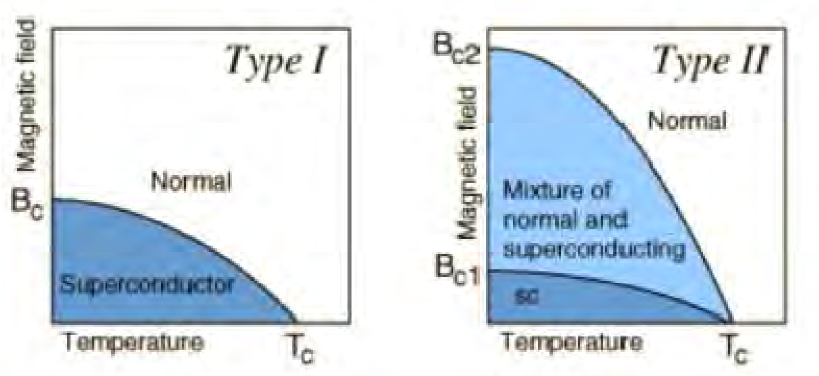


Figure1.2: Phase diagram of type I and type II superconductors

Source: http://hyperphysics.phy-astr.gsu.edu/HBASE/Solids...

1.3 Phenomenological and BCS theory

The theory of superconductivity has developed along two lines; the phenomenological and microscopic theory. The phenomenological treatment was initiated by F.London [7] who modified the Maxwell electromagnetic equation so as to allow for the Meissenr effect. His theory explained the existence and order of magnitude the penetration depth. The treatment was extended by V.L Ginzburg and L.D Landau and by A.B Peppered who in particular emphasized the concept of coherence length (ξ). A.A Abrikosov used these ideas to develop a model for alloy for superconductors. He showed that if the electronic structure of the superconductor were such that the coherence length becomes smaller than the penetration depth, on would get magnetic behavior similar to type II of superconductors, with two critical fields B_{c1} and B_{c2}.

The microscopic theory of superconductivity was initiated by H.Frohlich [8], who was first recognizing the importance of the interactions of electrons with lattice. Discovery of the isotope effect on T_c supported his assertion that the electron-phonon interaction plays an essential role in superconductivity.

The detailed microscopic theory was developed by John Barden, Leon cooper and John Schrieffer in 1957 [9]. Their theories of superconductivity became known as the BCS theory. In the BCS theory framework, superconductivity is microscopic effect which result from condensation of electron pair called cooper pair. A cooper pair is the name given to the electrons that are bound together in a certain manner and first discovered by Leon Cooper. Cooper showed such binding will occur in the presence of an attractive potential, no matter how weak.

In the BCS theory, a system of electrons is interacting with phonon which is the quantized vibration of the lattice. There is a screened coulomb repulsion between pairs of electrons, but in addition there is also attraction between them via the electron-phonon interaction. If the net effect of these two interactions is attractive, then the lowest energy state of the electron system has a strong correlation between pairs of electrons with equal and opposite momenta and opposite spin.

A simplified explanation of cooper pair formation: an electron moving through the conductor will attract the positive ions in the lattice. This attraction can distort the positively charged ions in such away as to attract other electrons (the electron-phonon interaction). The attraction due to the displace ion can overcome the electron repulsion due to the electrons having the same charge and cause them to pair.

BCS theory explored superconductivity at a temperature close to zero for elements and simple alloys (conventional) superconductors. However, at high temperature and with different superconductor system, the BCS theory has subsequently become inadequate to fully explain how superconductivity occurring.

1.4 HTS and its mechanism

After the discovery of superconducting mercury by Kamerlingh Onnes in 1911, the search for new superconducting materials lead to a slow increase in the highest known transition temperature(T_c) over the decades reaching a plateau at 23K with the discovery of superconducting of Nb_3Ge by Gavaler in 1973. After 13 more years, higher transition temperature was discovered in 1986 in 'LBCO'(a mixed oxide of lanthanum, barium, and copper) by Bendnorz and Muller, for which they were awarded the Nobel prize in 1987. The term high temperature superconductor was first used to designate for this newly discovered cuprate oxide. Another big jump to T_c about 90K followed quickly, with the discovery of "123" class of materials, exemplified by $YBa_2Cu_3O_7$-(YBCO), the Y(yttrium) can be replaced by many other rare earth elements example La, Nd, Sm and Gd with similarly high T_c. Shortly thereafter, still higher T_c values were found in the BSCCO (mixed oxide of bismuth, strontium, calcium and copper) and the"TBCCO" system (mixed oxides of thallium, barium calcium, and copper). In all of these systems, copper oxide planes form a common structural element, which is thought to dominate the superconducting property [10]. In the context of superconductivity, high superconductivity (high-Tc or HTS) are material that have a superconductivity transition temperature above the temperature historically been taken as the upper limit allowed by BCS theory. This is above the 1973 record of 23K that had lasted until copper- oxide materials were discovered [11].

Recently, iron- based superconductors with the critical temperature as high as 55K have been discovered. These are often also referred to as high- temperature superconductors. High-T_c superconductors (unconventional superconductors) differ in many important ways from conventional superconductors, such as mercury or lead, which are adequately explained by BCS theory. All known high-T_c superconductors are type II superconductors which allow magnetic fields to penetrate their interior in quantized units of flux, meaning that much higher magnetic fields are required to suppress superconductivity.

If we call, without strict definition, the superconducting materials with T_c exceeding the record value of 23K before 1986 as high-temperature superconductors (HTS), it's now realized in eight families of materials. Starting from the cuprates (1986), they are $Ba_{1-x}K_xBiO3$ (1988), intercalated C_{60} (1991), borocarbide (1994), HfNCl (1998), MgB_2 (2001), Ca under high-pressure (2006), and the newly discovered Fe pnictides (2008) [12].

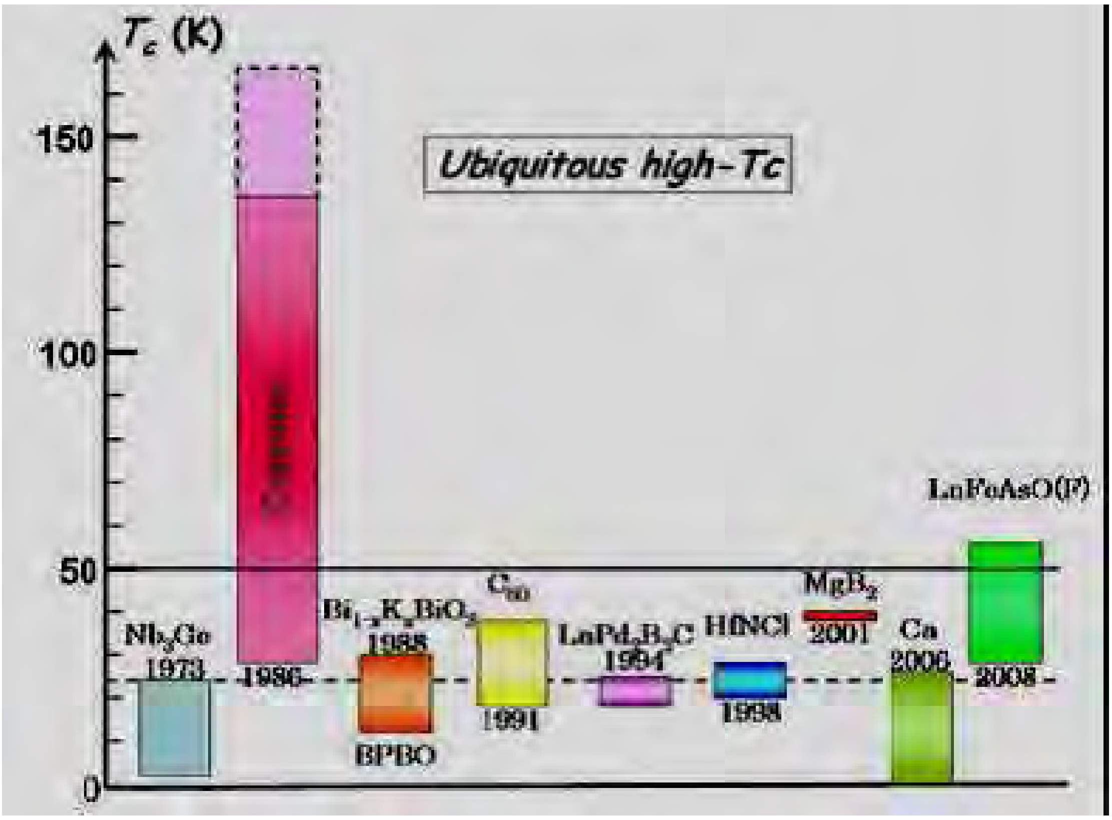


Fig. 1.3: High-temperature superconducting materials

discovered since 1986 and their critical temperatures (*Tc*).

The mechanism of superconductivity is one of the most exciting areas in the study of high-T_c superconductors. Understanding the mechanism superconductivity will clarify how magnitude of T_c can reach and how it may be pushed higher, as well as why its pressure dependence is so large [8]. The mechanism that causes the electrons to form pairs in high-temperature superconductors is not clearly known. However, lattice vibrations alone are not strong enough to maintain electron pairing at elevated temperatures. Pairing mechanisms of magnetic origin have been proposed, mainly to justify the high critical temperatures of HTS: the magnetic exchange energies are about four times the phonon energies. In this case, the electron pairing would have a wave function with d-wave symmetry. One of the most dominant theories that contain d-wave symmetry is the spin wave model. According to this theory, the carrier leaves a magnetic disturbance (a spin wave) in its wake. This wake pulls a second carrier, so that the two forms a Cooper pair. The spin waves are short lived, so they are often called spin fluctuations [13]. Thus, determining whether the pairing wave function has d-wave symmetry is essential to test the spin fluctuation mechanism. In addition to d-wave symmetry the pairing symmetry can be an extended s- wave, p- wave might be result of the spin fluctuation mechanism. Pairing symmetry provides clues to the identity of the superconducting pairing mechanism which is essential for the development of the theory of high temperature superconductivity. In general possible orbital pairing states include s-wave, an extended s-wave, p-wave and d-wave states. In the s-wave state, the energy gap $\Delta(\mathbf{k})$ is isotropic; i.e., $\Delta(\mathbf{k})$ is constant over the Fermi surface.

1.5 Superconductivity and magnetism in Fe-pnictide superconductors

The recently discovered quaternary arsenide oxide superconductor $La(O_{1-x}F_x)FeAs$ with the superconducting critical transition temperature (Tc) of 26K, has been quickly expanded to another family of high-Tc superconducting systems besides copper oxides by the replacement of La with other rare earth elements. One of the superconductors that obtained replacing La by Sm is samarium-arsenide oxides $Sm(O_{1-x}F_x)FeAs$ with a critical temperature Tc of 55K, which is the highest among all materials besides copper oxides up to now [14]. A superconductivity in Neodymium arsenide oxides $Nd(O_{1-x}F_x)FeAs$, with the onset resistivity transition at 51.9K and Meissner transition at 51K was synthesized by replacement of La with Nd which is also non-cuprate compound that superconductors above 50K. The other discovered bulk superconductivity is in the praseodymium arsenide oxides $Pr(O_{1-x}F_x)FeAs$ with an onset drop of resistivity as high as 52K is also obtained by substitution of La by Pr. Replacement of La by Ce, leads to a large increase in critical temperature (T_c) from 26K to

41K in layered $CeO_{1-x}F_xFeAs$. The superconductivity has been also discovered in oxygen free AFe_2As_2 (*A*=Ba, Sr, Ca) [15].

Like the cuprates, the pnictides are highly two dimensional, their parent material shows spin density wave (SDW) order below 150K, and superconductivity occurs upon doping of either electrons or holes into the FeAs layers. There is a growing consensus among researchers that Mott physics does not play a significant role for the iron pnictides, which remain itinerant for all doping levels, including parent compounds, in which magnetic order is of spin-density wave (SDW) type rather than Heisenberg antiferromagnetism of localized spins. This is evidenced by, e.g., a relatively small value of the observed magnetic moment per Fe atom, which is around 12–16% of $2\mu_B$ [15]. The cause of the spin density wave which is a type of antiferromagnetic is associated with structural phase transition from tetragonal to orthorhombic. Cruz et al. Neutron-scattering experiments reveal that a structural phase transition in LaFeAsO is at T_S~155K where T_s is structural transition temperature. This result demonstrates that LaFeAsO undergoes an abrupt structural distortion below 155K, and the symmetry changes from tetragonal (space group P4=nmm) to orthorhombic (space group Cmma) at low temperatures. Further more, they carried out order parameter measurements to determine whether or not the ordered magnetic scattering at low temperatures in LaFeAsO is indeed associated with structural-phase transition. And they found the ordered magnetic moment vanishes at temperature~137K, approximately ~18K lower than the temperature at which the structural phase transition occurs. Therefore, the magnetic anomaly at approximately 150K is caused by structural distortion. In contrast, neither structural nor magnetic anomaly was observed in superconducting state [18]. The La-NMR experiment result has also shown that the magnetic ordering is related to the structural distortion. The structural phase transition have seen in other pnicted such as SmOFeAs, CeOFeAs and so on with different T_s. Experiments and theoretical calculations suggest that ROFeAs exhibits a spin-density-wave (SDW) instability that is suppressed by doping with electrons to induce superconductivity, but there has been no direct evidence of SDW order [16].

1.6 Crystal structure of Fe-pnictide superconductors

The layered iron superconductors, discovered by Kamihara and co-workers [17], now comprise a rather large family of materials, with four distinct crystallographic types. The first one is RFeAsO (R=rare earth element) which is called the "1111" structure (space group P4=nmm). Figure 1.4 below shows the first type of crystal structure. The RO and FeAs layers are stacked along the c-axis. The first discovered iron-pnictide superconductor LaFeAs($O_{1-x}F_x$) has this structure, and various rare-earth elements such as Sm, Ce, Pr, and Nd can enter the R site [18]. The experimental lattice parameters for LaFeAsO are a=4.03552Å, c=8.7393Å [19]. For the undoped SmOFeAs, the lattice parameters a=3933(5)Å, c=8.495(4)Å[14], for the undoped CeOFeAs, a=3.996Å,c=8.648Å [20] and so on. The Fe atoms form a planar square lattice which is sandwiched by As square lattice or two-dimensional network of $FeAs_4$ tetrahedra is formed. The FeAs layer is a conduction plane for charge carriers and a main stage of superconductivity. The other building block $RO_{1-x}F_x$ is a charge reservoir layer, controlling the carrier density or chemical potential [12]. The unit cell contains two molecules, and the chemical formula is represented by (La_2O_2)(Fe_2- As_2). The Fe_2As_2 layer, which is sandwiched between the La_2O_2 layers, serves as a carrier conduction path. Thus, conduction carriers are two-dimensionally confined in the Fe_2As_2 layer, causing strong interactions among the electrons. All iron-pnictide supercondu-ctors are layer with tetragonal structure at room temperature.

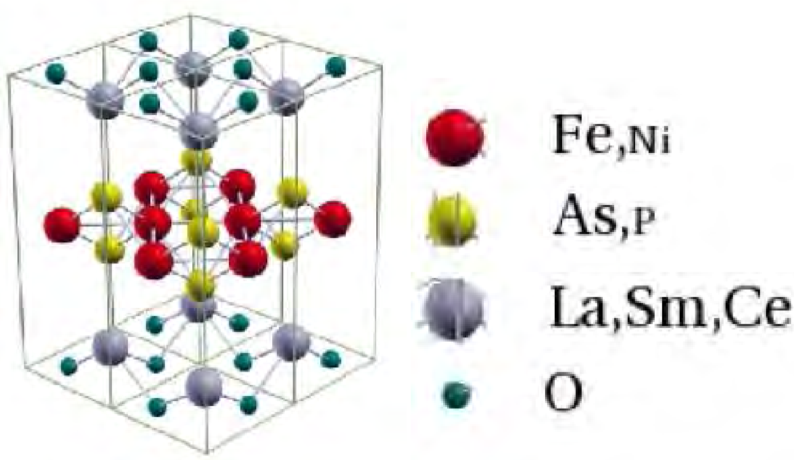


Figure 1.4: Tetragonal structure of ROFeAs

The second iron-pnictide family is abbreviated as "122", and is well-known in "heavy-fermions (HF)"compounds. The third structure was reported in superconducting LiFeAs, called the "111"structure. LiFeAs crystallizes into the Cu_2Sb-type tetragonal structure containing the FeAs layer with an average iron valence of +2 like those for the "1111"or"122" parent compound. Recently, superconductivity has been reported at 8K in ∝ -FeSe compounds with the ∝ -PbO-type structure. This structure, shortened as the "11"structure [18].

1.6.1 Electronic structure Fe-pnictide superconductors

To understand the bulk electronic properties in the metallic state of RFeAsO, it is important to determine electronic structure. The electronic structure proposed by band-structure calculations and supported by angle-resolved photoemission spectroscopy (ARPES) consists of two small hole pockets centered around Γ point **p**= (0, 0) and two small electron pockets centered around *M* point **p**=**Q**= (π,π) in the folded Brillouin zone (BZ)[15].

The Fermi surfaces of the undoped LaFeAsO were discussed on the basis of the results of the density functional studies by Singh and Du [19] has five sheets: two high velocity electron cylinders around the zone edge *M-A* line, two lower velocity hole cylinders around the zone center, and an additional heavy 3D hole pocket, which intersects and anticrosses with the hole cylinders, and is centered at *Z*. The heavy 3D pocket is derived from Fe d_z states, which hybridize sufficiently with As *p* and La orbitals to yield a 3D pocket. The remaining sheets of Fermi surface are nearly 2D. The electron cylinders are associated with in-plane Fe *d* orbitals and have higher velocity and will make the larger contribution to the in plane electrical conductivity.

As an important feature of the Fermi surfaces in these compounds, the cylinders at the Γ and M points are nearly nested and can yield strong nesting peaked at (π,π) in the folded Brillouin zone (two Fe atoms in the unit cell). This can lead in general to enhanced spin fluctuations in this nesting vector and, if these fluctuations are sufficiently strong, they can cause stripe-type spin-density-wave (SDW) ordering. From similar band calculations in other transition metal pnictides RTAsO (T =Cr, Mn, Co, and Ni), it was found that the Fermi surface nesting only occurs in RFeAsO, which makes RFeAsO distinct from the others [18]. The electronic states near the Fermi level are formed dominantly by the Fe3d electronic states. Thus, iron pnictides may be considered to be typical strongly correlated electron systems, in which the strong Coulomb interaction among the iron 3d electrons can affect the electronic properties significantly. The Fermi surface consists of hole pockets around the Γ point and electron pockets around the M point, qualitatively consistent with the results of angle-resolved photoemission (ARPES) experiments and more recent quantum oscillation-experiments [21]. Although the lattice structure is similar to the cuprates, the basic electronic structure is quite different. The electronic states near the Fermi level are composed of mainly Fe 3d orbitals. All the five 3d orbitals contribute to form closely separated electronic bands with various electron– and hole-Fermi sheets (pockets). Thus, the Fe compounds are a multi-band system in contrast to the single-band system of the cuprate [12].

1.7 Physical Properties $R(O_{1-x}F_x)FeAs$

The superconductivity in the high T_c cuprate arises from either electron or hole doping in the non superconducting parent compounds. The parent material shows anomalies such as in resistivity. Owing to this, some researchers share the view that in so far as the normal state properties reflect the electronic structure that underlies high T_c superconductivity, it is necessary to develop an understanding of the normal state before the superconducting state can be understood.

Superconductivity in the newly discovered rare-earth iron-based oxide systems ROFeAs (R=La, Ce, Nd, Pr and Sm) also arises from either electron or hole doping of their non-superconducting parent compounds. The parent material LaOFeAs is metallic but shows anomalies near 150K in both resistivity and D.c. magnetic susceptibility [22].

Dong et al. investigated the systematic F-content dependence of the electrical resistivity of $LaFeAs(O_{1-x}F_x)$, which is shown in Fig below. The resistivity of undoped LaFeAsO shows weak temperature dependence with a high value at high temperatures, and exhibits a steep drop at approximately150K with an upturn below 50K. The resistivity of the 2% F-doped sample decreases and the 150K anomaly shifts to a lower temperature and becomes less pronounced. In the 3% F-doped sample, no anomaly was observed and a superconducting transition occurs at 17K. With further F doping, superconducting-transition temperature increases and leads to the highest T~28K for 10% F doping [18].

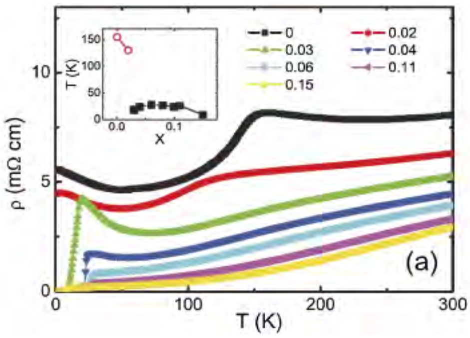


Fig.1.5: Temperature dependence of electrical resistivity of LaFeAs ($O_{1-x}F_x$).

The measurements in LaFeAs ($O_{1-x}F_x$) by Kohama et al. [23] and Klingeler et al. [24] was revealed that the x_{bulk} of LaFeAs ($O_{1-x}F_x$) is independent of local-moment effects by rare-earth elements, and is affected only by the iron 3d electrons. In both reports, the x_{bulk} of LaFeAsO shows a gradual decrease from room temperature and exhibits a small drop at T_S where the structural transition occurs. Below approximately 50K, X_{bulk} shows an upturn behavior, which would be ascribed to an impurity contribution. The temperature dependences of the X_{bulk} of the F-doped compounds are different between the above two reports. The bulk of the F-doped sample reported by Kohama et al. shows an increasing behavior with decreasing temperature, but that reported by Klingeler et al. shows a gradual decrease with decreasing temperature as in the undoped LaFeAsO. Since the temperature dependence of the As-Knight shift is scaled to the latter behavior, the former temperature dependence is considered to be significantly affected by impurity phases. Klingeler et al. also reported that the temperature dependences of X_{bulk} well above T_N and T_c are barely unchanged in a wide doping region, although the ground state changes from an orthorhombic spin density wave(SDW)/antiferromagnetic poor metal to a tetragonal nonmagnetic superconductor upon F doping [18]. In addition, susceptibility for 5 atom % F-doped sample starts to decrease at ~25K and shows large negative values with the lowering of *T*. On the other hand, mol susceptibility T for the undoped sample shows positive values in the entire temperature range examined. The zero resistivity and the large diamagnetic susceptibility show that LaOFeAs becomes a superconductor by F-doping [4].

Standard 4-probe DC resistivity and AC susceptibility measurements show that, the pure CeOFeAs sample has rather high dc resistivity value. The resistivity increases slightly with decreasing temperature, but below roughly 145K, the resistivity drops steeply. After *F* doping, the overall resistivity decreases and the 145K anomaly shifts to lower temperature and becomes less pronounced. At higher *F* doping, the anomaly disappears and a superconducting transition occurs. The resistivity behavior of the pure CeOFeAs is very similar to that of LaOFeAs, except that a resistivity up turn was observed in the later compound at low temperature. As we saw earlier, the anomaly at 150K is caused by spin-density-wave instabilit. The direct current magnetic susceptibility measurement of the parent CeOFeAs revealed that magnetic moment per formula unit is 2.43μ_B, which is close to the magnetic moment of free Ce_{3+} ion [20].

The same experimental method measurement in Nd[O1-xFx]FeAs show that a clear resistivity drop as the temperature is down to 51.9K, and the resistivity was unmeasurable below 48.8K. The middle of the superconducting transition is at 50.1K. Comparing with $Pr[O_{0.89}F_{0.11}]FeAs$ superconductor, the *Tc* (zero) increases about 5K while the *Tc*(onset) has no obvious change. The sharp magnetic transitions on both of AC and DC susceptibility curves that measured experimentally indicate the good quality of this superconducting component [25].

The standard four-probe method in a physical property measurement system Pr[O1-xFx] show that the zero-field resistivity shows a clear drop as the temperature down to 52K, and becomes unmeasurable at 44K. The middle of the superconducting transition is 47K [26].

The resistivity of SmOFeAs shows an anomaly at 150K, which is similar to that of other ReOFeAs compounds, and this anomaly was confirmed to be caused by the occurrence of spin density wave instability. For the $Sm[O_{0.9}F_{0.1}]FeAs$, the temperature of the onset resistivity transition was found to be at 55.0K and the zero resistivity appeared at 52.6K, which is higher than that of Pr[O1-xFx]FeAs and $Nd[O_{1-x}F_x]FeAs$, and then becomes the highest among all superconducting materials besides copper oxides. As Sm has a smaller covalent radius comparing with La, Ce, Pr and Nd, the inner chemical pressure that caused by the shrinkage of crystal lattice is thought to be an important factor that enhances *Tc,* as proposed in a theoretical calculation, where it is indicated that the *Tc* may be enhanced by the increase of hopping integral, which can be achieved by the shrinkage of the lattice. The sharp magnetic transitions on the DC susceptibility curves measurement indicate the good quality of this superconducting component. The onset diamagnetic transition starts at 54.6K [14].

1.8 Mechanism of superconductivity in Fe-pnictide

In the Bardeen-Cooper-Schrieffer theory of superconductivity, electrons form Cooper pairs through an interaction mediated by vibrations of the crystal. Like lattice vibrations, magnetic fluctuations can also produce an attractive interaction creating Cooper pairs, though with spin and angular momentum properties different from those of conventional superconductors [25]. The newly discovered iron-pnictid superconductor is unconventional superconductivity such as that in copper oxides. The reasons why unconventional pairing may be realized in iron pnictides: (i) T_c is very high, compared with conventional phonon-mediated BCS superconductors (ii) electron-phonon coupling is expected to be weak according to first-principles calculations [21].

Up to now, many theoretical studies of the iron-pnictid superconductors have been reported. As for the superconducting pairing state, most of them have proposed the s pairing state. Here, we introduce some of the works suggesting the s ± pairing state, which were reported just after the discovery of the superconductors. A.V.Chubukov et al. suggest that both magnetic and pairing instabilities are determined by the same interband pair hopping which transforms two fermions near the hole Fermi surface (FS) into two fermions near the electron Fermi surface (and vice versa). When electron and hole pockets are nearly identical, spin density wave(SDW) instability occurs at a higher *T*. When the near identity is broken by either hole or electron doping, the Cooper instability comes first. This pairing interaction sets the gaps in hole and electron pockets to be of equal magnitude Δ, but of opposite signs (an extended *s*-wave symmetry, *s*+) [15].

Ding et al. have performed ARPES measurements on the Superconducting iron pnictide and two superconducting gap without node were observed on small hole-like and electron-like

Fermi surface sheets. They suggest that the pairing mechanism originates from the inter-band interactions between these two nested Fermi-surface sheets. Similar experimental results from different groups on the "1111" system have been reported and they strongly suggest that a) the superconducting gap is nodeless, which excludes the p-wave and d-wave pairing states with nodes of the gap on the Fermi surfaces but consistent with s wave pairing, and that b) the magnitude of superconducting gap is orbital-dependent. Nodeless superconducting gap was also suggested from magnetic penetration-depth measurements. Hashimoto et al. Magnetic penetration-depth measurements on underdoped single crystals of $PrFeAsO_{1-\delta}$ (T_c =35 K), suggests a nodeless superconducting gap. A similar two-nodeless gap model is also applied in $SmFeAsO_{1-x}F_x$ (T_c = 45 K), but the result suggesting a single fully gapped order parameter with a small anisotropy reported in single crystals of $NdFeAsO_{1-x}F_x$(x=0.1).

Mazin et al. argued that superconductivity realized in the iron-pnictide compounds is unconventional and mediated by antiferromagnetic spin fluctuations. Its pairing state is an extended s-wave pairing with a sign reversal of the order parameter between different Fermi surface sheets [26]. They claimed that doped LaFeAsO represents the first example of multigap superconductivity with a discontinuous sign change in order parameter between the bands. Their scenario is based on the calculated Femi surfaces for the undoped LaFeAsO, and the superconductivity is induced by the nesting-related antiferromagnetic spin fluctuations near the wave vectors connecting the electron and hole pockets.

Kuroki et al. [27] constructed a minimal model, where all the necessary five d-bands are included and calculated spin susceptibility and charge susceptibility within random phase approximation. Furthermore, they investigated superconducting properties using the linearized Eliashberg equation, and concluded that the multiple spin-fluctuation modes arising from the nesting across the disconnected Fermi surfaces realize an extended s-wave pairing, in which the gap changes sign between the hole and electron Fermi surfaces across the nesting vector. This unconventional s-wave pairing is the same as the s ±state proposed by Mazin et al.. Kuroki et al. also suggest that a dx^2-y^2-wave pairing, in which the gap changes sign between the electron Fermi surfaces, can also be another candidate, if the hole Fermi surfaces around Γ are absent (or less effective). To identify the mechanism of iron-pnictide superconductivity, the determination of the presence or absence of nodes in the superconducting gap is quite important.

1.8. 1 Effect of F-doping in ROFeAs

To achieve superconductivity, two methods are commonly used, doping and applying pressure. Either electron doping or hole doping can introduce superconductivity. In the cuprates doping is necessary for introducing mobile charge carriers, since the parent compounds are Mott-Hubbard insulators. Superconductivity in the newly discovered rare-earth iron-based oxide systems ROFeAs (R is rare-earth metal) also arises from either electron or hole doping of their non-superconducting parent compounds. Since the parent material ROFeAs is metallic, and doping does not appear to change the charge density very much. F-ion substitution for the O sites changed the bond length and bond angle in the distorted LaO tetrahedron, whereas weaker geometric effects were observed in the FeAs layer. Further, the F-doping induced large decreases in the c-axis length and the La-As distance, suggesting an enhancement of the polarizations in the $(LaO)^{\delta+}$and $(FeAs)^{\delta-}$ layers as a result of electron transfer between two layers. The enhanced polarization and Fe-Fe interaction in the FeAs layer are likely to suppress the transition leading to the emergence of superconducting phase. In general, the effect of F-doping at the O sites are summarized as follows : a) the F-doping acts as an electron donor, leading to a supply of the extra electrons to the FeAs layer, which results in a shift of the chemical potential to lower binding energy side. b) the c-axis length and La-As distance are shortened as result of the enhancement of the charge polarization of the $(LaO)^{\delta+}$and $(FeAs)^{\delta-}$layers. C) the Fe-Fe distance decreases, which may enhance the interaction among 3d electrons. d) the distortion of the La_4O tetrahedron is relaxed largely, whereas less structural changes take place in the FeAs tetrahedron. It is likely that interplay of these effects may prohibit the crystallographic and magnetic transitions to occur and generate the superconducting phase [28]. The effects of F-doping observed in LaO1-xFxFeAs are also observed in other rare earth compound. Experimental measurement shows that the F doping iron pnictide have smaller lattice parameter as compared to the parent compound. For example, the lattice parameter for the parent CeOFeAs and $CeO_{1-x}F_xFeAs$ x=0.16 of F doping compound obtained a =3*:*996Å , c = 8*:*648Å , and a = 3*:*989 Å, c=8*:*631 Å respectively. Compared to the undoped phase CeOFeAs, the apparent reduction of the lattice volume upon F doping indicates a successful chemical substitution. For the undoped SmOFeAs, the lattice parameters a = 3.933(5) Å, c =8.495(4) Å, while all superconducting samples have smaller lattices; for the nominal $Sm[O_{0.9}F_{0.1}]FeAs$, a = 3.915(4) Å and c = 8.428(7) Å [14]. This result is similar to other rare earth substitutions, and indicates the covalent character of the intra-layer chemical bonding due to the smaller covalent radius of fluorine than oxygen.

1.9. Spin Density Wave

Spin-density wave (SDW) occurs at low temperature in anisotropic, low-dimensional materials or in metals that have high densities of states at the Fermi level $N(E_F)$. Other low-temperature ground states that occur in such materials are superconductivity, ferromagnetism and antiferromagnetism. Experimental investigations show that the SDW is a kind of antiferromagnetic state, with the electronic spin density forming a static wave. The density varies periodically as a function of position with no net magnetization in the entire volume. The SDW transition occurs when the spatial spin density modulation is due to delocalized or itinerant electrons rather than localized ones.

In normal state the density $\rho_{\uparrow}(r)$ of electrons spins polarized upward cancelled by density $\rho_{\downarrow}(r)$ of dowenward polarized spins. In the SDW state, however, the difference between $\rho_{\uparrow}(r)$ and $\rho_{\downarrow}(r)$ is finite and undulates in space as a function of position vector r in the SDW state [8]. SDW ground state is obtained from the single band Hubbard model with in the Hartree-Fock approximation and assuming that the nesting of the Fermi surface exists only in certain direction of the Fermi surface. The direction of the Fermi surface where nesting exists will be instable with respect to the SDW formation whereas the superconductivity instability may occur in the rest of the part of the Fermi surface, provided there exists some attractive interaction between the quasi particles mediated by some boson exchange. Therefore, one can present a model to study the coexistence of superconductivity and SDW, that incorporates two competing physical processes involving electron-hole spin density wave(SDW) like pairing of opposite spins with a net momentum difference (Q) between the conjugates and electron-electron (superconducting) pairing of opposite spins with total momentum zero.

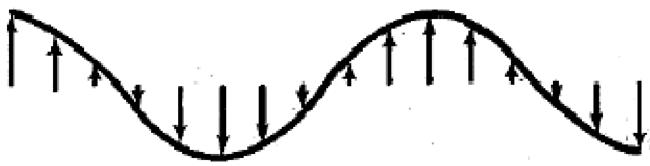


Fig.1.6: Spin density wave

1.10 The coexistence of superconductivity and magnetism

The interplay of magnetism and superconductivity is a fundamental problem in condensed matter physics. These two phenomena were thought mutually antagonistic. In conventional superconductors (BCS theory of superconductivity), local magnetic moments break up the spin-singlet Cooper pairs and hence strongly suppress superconductivity , an effect known as pair-breaking. Typically, magnetic fields destroy superconductivity because the energy they generate perturbs the close interaction between pairs of electrons that is a prerequisite for superconductivity. The most common way that a magnetic field destroys superconductivity is by disturbing the orbital effect, where the electrons in a pair orbit each other, acquiring more and more energy from the magnetic field. Once this energy becomes greater than that which unites the two electrons, the electron pairs break apart and superconductivity is suppressed. The other way magnetic fields can destroy superconductivity is when two electrons have what is called opposite spin; this is when in addition to the two electrons orbiting one another, they also are spinning like tops but in opposite directions, called s-wave spin. When the magnetic field is turned on, one electron gains energy while the other loses. "If the difference is bigger than the amount of energy holding the electrons together, then they fly apart and superconductivity has gone," explained Naughton [29].

However, in a limited class of inter-metallic systems, superconductivity occurs even though magnetic ions with a local moment occupy all of one specific crystallographic site, which is well isolated and de-coupled from the conduction path. The possible coexistence of superconductivity with various types of magnetism carried by localized magnetic moments and itinerant electrons is critically discussed in connection with several existing materials such as rare earth ternary compounds [(RE)Mo_6S_8, (RE=Gd,Tb,Dy and Er) (RE)Mo_6Se_8 and (RE)Rh_4B_4], (RE=Nd ,Sm and Tm magnetic system[30], and has been recently revitalized by the discovery of the RNi_2B_2C(R=Y,Tm,Ho and Dy) system. In all three systems, both SC and antiferromagnetic (AFM) ordered states coexist.

The coexistence of superconductivity and ferromagnetism in the same compound has been put forward theoretically by V. Ginzburg in 1957 [31]. In his theoretical explanation, the coexistence of magnetism and superconductivity occurs when ferromagnetic field is smaller than the thermodynamic critical field of superconductor. The coexistence of superconductivity and antiferromagnetism is quite peaceful and very weakly influences each other, because the antiferromagnetic molecular field is effectively averaged out within the scale of the superconducting coherence length. Superconductivity coexisting with ferromagnetic order was recently observed in UGe_2 and URhGe. This superconducting phase is found within the ferromagnetic phase and disappears in the paramagnetic region. The coexisting superconductivity with ferromagnetic is strongly suggesting that the pairing mechanism is magnetic in origin [32]. Experimental study on the newly discovered iron pnictide superconductor found that magnetism and superconductivity coexists in the long rang doping in $SmO_{1-x}F_xFeAs$ ($0.1 \leq x \leq 0.13$) [33].

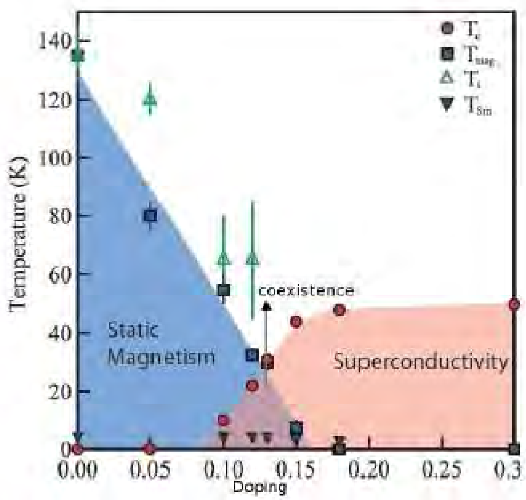


Figure 1.7: Phase diagram with fluorine doping inSmFeAs01-xFx

Recently, Muon Spin Relaxation measurement revealed that superconducting and magnetic phases coexists in $LaFeAs(O_{1-x}F_x)$ with x=0.06(Tc ≈ 18 K) [34]. These two phase indeed coexist in the form of macroscopic phase separation, and more interestingly, that a spin glass-like magnetic phase develops in conjunction with superconductivity in the paramagnetic phase. This accordance strongly suggests a common origin of the electronic correlation leading to these two competing phases.

Chapter 2

Mathematical Methods

2.1 Introduction

To study the coexistence of superconductivity and spin density wave (SDW) in $SmO_{1-x}F_xFeAs$ theoretically we have used Green's function technique. Green's function play an important role to solve inhomogeounes differential equation subjected to boundary condition. The term is used in physics especially in quantum field theory, electrodynamics and statistical field theory, to refer to various types of correlation functions, even those that do not fit the mathematical definition. The methods of quantum field theory, which is successfully applied to elementary particle physics, provide a very powerful and unified way of attacking the many body problems. To deal with the many body problems, the first step expresses the Hamiltonian of a system in terms of creation and annihilation operators. In many body, the term Green function is sometime used interchangeably with correlation function, but refer specifically to correlates field operators or creation and annihilation operators.

2.2 Green's function formalism

In quantum field theory Green's functions are called propagators. This name is based on the idea that, in order to find the important physical properties of the system, it is essential to know, not detailed behavior of each particle in the system, but the average behavior of one or two typical particles. The quantities that described this average behavior are called the one and the two particle propagator respectively. There are many types of Green' function: one particle, two particles… n-particles, the double time causal, retarded, advanced Green's function and so on. In this work we have used double time dependent Green's function in particular the double time retarded [35]. The double time dependent retarded Green function is equal to the change of the average value of some dynamic quantity by the time t.

The double time retarded and advanced Green's functions are defined respectively as

$$G_r(t-t') = \ll \hat{A}(t), \hat{B}(t') \gg_r = -i\Theta(t-t') <[\hat{A}(t), \hat{B}(t')]>, \quad (2.1)$$

$$G_a(t-t') = \ll \hat{A}(t), \hat{B}(t') \gg_a = i\Theta(t-t') <[\hat{A}(t), \hat{B}(t')]>. \quad (2.2)$$

Where $\ll \cdots \gg$ is abbreviated notation for the corresponding the Green's function and < > indicates the average over a grand canonical ensemble for the operators. $\Theta(t-t')$ is Heaviside step function, $\hat{A}(t), \hat{B}(t')$ are operators in Heisenberg picture.

$\hat{A}(t)$ can be written as;

$$\hat{A}(t) = \exp(iHt)\, A(0) \exp(-iHt). \quad (2.\ 3)$$

And

$$\Theta(t,t') = \begin{cases} 1, t > t' \\ 0, t < t' \end{cases}$$

$[\hat{A}(t), \hat{B}(t')]$ is the commutator or anti-commutator. This is expressed as,

$[\hat{A}(t), \hat{B}(t')] = \hat{A}(t)\hat{B}(t') - \tau\, \hat{B}(t')\, \hat{A}(t)$.

Where $\tau = 1$ for bosons and $\tau = -1$ for fermions.

To find the equation of motion for the Green's function differentiating eq. (2.1) with respect to time and, we get

$$\frac{dG(t-t')_r}{dt} = \frac{d}{dt} \ll \hat{A}(t), \hat{B}(t') \gg \quad (2.4)$$

$$\frac{dG_r(t-t')}{dt} = -\frac{d}{dt}\, i\Theta(t-t') < \left[\hat{A}(t), \hat{B}(t')\right] > \quad (2.5)$$

$$\frac{dG_r(t-t')}{dt} = -\frac{d}{dt}\, i\Theta(t-t') < \left[\hat{A}(t), \hat{B}(t')\right] > -i\,\Theta(t-t') < \frac{d}{dt}\left[\hat{A}(t), \hat{B}(t')\right] > \quad (2.6)$$

multiplying eq. (2.6) by i, we get

$$\frac{idG_r(t-t')}{dt} = \frac{d}{dt}\, \Theta(t-t') < \left[\hat{A}(t), \hat{B}(t')\right] > -i\,\Theta(t-t') < \left[i\frac{d}{dt}\, \hat{A}(t), \hat{B}(t')\right] > \quad (2.7)$$

$$\frac{idG_r(t-t')}{dt} = \frac{d}{dt}\, \Theta(t-t') < [\hat{A}(t), \hat{B}(t') > + \ll i\frac{d}{dt}\, \hat{A}(t), \hat{B}(t') \gg. \quad (2.8)$$

The relation between Heaviside step function Θ(t) and Dirac delta function δ is given by

$$\Theta(t) = \int_{-\infty}^{t} \delta(t)dt.$$

The equation of motion expresses as,

$$\frac{id\hat{A}(t)}{dt} = [\hat{A}(t), \hat{H}],$$

we consider, ħ = 1.

Thus, eq. (2.8) can be written as;

$$\frac{idG_r(t-t')}{dt} = \delta(t-t') < [\hat{A}(t), \hat{B}(t')] > + \ll [\hat{A}(t), H], \hat{B}(t') \gg . \tag{2.9}$$

We can write the above expression as

$$\frac{idG_r(t-t')}{dt} = < [\hat{A}, \hat{B}] > + \ll [\hat{A}, H], \hat{B} \gg .$$

In order to solve eq. (2.9), it is convenient to use Fourier transformation of this equation. The function depend on time t and t' through $(t - t')$. Therefore we can use G$(t - t')$ in the place of G (t, t').

Let $G_r(\omega)$ represents the Fourier transformation of $G_r(t - t')$ and the relation is given by,

$$G_r(t-t') = \int_{-\infty}^{\infty} G_r(\omega)\, e^{-i\omega(t-t')}\, d\omega \tag{2.10}$$

and

$$G_r(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G_r(t-t')\, e^{i\omega(t-t')} dt. \tag{2.11}$$

The delta function δ is define by

$$\delta(t-t') = \int_{-\infty}^{\infty} e^{-i\omega(t-t')} d\omega. \tag{2.12}$$

From eq. (2.10), we obtain

$$\frac{dG_r}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} G_r(\omega)\, e^{-i\omega(t-t')} d\omega$$

$$\frac{dG_r}{dt} = -i\omega \times G_r(\omega)$$

Using the above expression, eq. (2.9) can be expressed as

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

$$\omega << \hat{A},, \hat{B} >> = <[\hat{A}, \hat{B}]>_\omega + << [\hat{A}, H], \hat{B} >>_\omega . \tag{2.13}$$

Here, $<<\hat{A},,\hat{B}>>$ denotes the Fourier transform of Green's function involving the operators A and B, it satisfies the equation of motion (2.13), where the double angular brackets $\ll \cdots \gg$ indicates the Green's function. The single brackets $< \cdots >$ indicates the thermal average over the canonical, that is

$$< F > = \frac{Trexp(-\beta H)F}{Trexp(\beta H)}.$$

Where $\beta = \frac{1}{K_\beta T}$, K_β is the Boltzmann constant

From the analytical properties the green functions it follows that the correlation functions $<\hat{B}(t'),\hat{A}(t)>$ can be obtained from the equation;

$$< \hat{B}(t'),\hat{A}(t) >= \lim_{\epsilon\to 0}\int_{-\infty}^{\infty}\frac{\ll \hat{A},\ \hat{B}\ \gg_{\hbar\omega+i\epsilon} - \ll \hat{A},\ \hat{B}\ \gg_{\hbar\omega-i\epsilon}}{\exp(\beta\hbar\omega)-1}e^{-i\omega(t-t')}\mathrm{d}\omega \qquad (2.14)$$

Chapter 3

FURMULATION OF THE PROBLEM

3.1 The coexistence of superconductivity and spin density wave (SDW) in $SmO_{1-x}F_xFeAs$

The muon spin rotation experiment revealed that superconductivity and spin density wave(SDW) both coexist in $SmO_{1-x}F_xFeAs$ in the range of 0.1< x < 0.13. The experiment has also confirmed that the magnetism originates from FeAs layer and is not associated with Sm ions, which order at much lower temperature [34]. The FeAs layer is also responsible superconductivity. Theoretical studies have shown the coexistence of superconductivity and magnetism in iron-based superconductors by considering a model of Hamiltonian. In this part of the study, we investigate the theoretical coexistence of superconductivity and SDW in $SmO_{1-x}F_xFeAs$. For this purpose, we tried to find the mathematical expression for the superconducting critical temperature (T_c), superconducting order parameter (Δ_{sc}) the magnetic order parameter (M) and SDW transition temperature (T_{sdw}).

3.2 Mathematical Formulation of the problem

The model of the Hamiltonian for coexistence SDW and superconductivity in our compound can be describe as

$$H = \sum_{p\sigma} \epsilon_p \, \hat{a}^+_{p\sigma}\hat{a}_{p\sigma} + M\sum_{p}\left(\hat{a}^+_{p+q\uparrow}\hat{a}_{p\downarrow} + \hat{a}^+_{p\downarrow}\hat{a}_{p+q\uparrow}\right) + \Delta_{sc}\sum_{p}\left(\hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right). \quad (3.2.1)$$

Where ($\hat{a}^+_{p\sigma}\hat{a}_{p\sigma}$) are the creation (annihilation) operator of an electron having the wave number k and spin σ. The superconducting order parameter (Δ_{sc}) and the SDW order parameters (M) are given by respectively as

$$\Delta_{sc} = -V\sum_k < \hat{a}_{-k\downarrow}\hat{a}_{k\uparrow} > = -V\sum_k < \hat{a}^+_{k\uparrow,}\hat{a}^+_{-k\downarrow} >,$$

$$M = -U\sum_k < \hat{a}^+_{k\uparrow,}\hat{a}_{k-q\downarrow} >.$$

To determine the order parameters, we first described the equation of motion.

We have to use the following property to solve the commutation relation.

[A, BC] = [A, B]C +B[A,C], for bosons,

[A, BC] = {A, B}C − B{A,C},for fermions.

We also apply the following anticommutation relation to solve the equation of motion.

$$\{\hat{a}^+_{k\sigma}\hat{a}_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}\ and\ \{\hat{a}^+_{k\sigma}\hat{a}^+_{k'\sigma'}\} = \{\ \hat{a}_{k\sigma}\hat{a}_{k'\sigma'}\} = 0,$$

$[\hat{a}_k\hat{a}^+_{k'}] = \delta_{kk'} = 1\ if\ k = k'$ otherwise zero

and $\delta_{\sigma\sigma'} = 1$ if $\sigma = \sigma'$ otherwise zero.

3.2.1 The superconducting order parameter

The equation of motion for the correlation $\ll \hat{a}^+_{k\uparrow,}\hat{a}^+_{-k\downarrow} \gg$ to describe the superconducting order parameter can be written as;

$$\omega \ll \hat{a}^+_{k\uparrow,}\hat{a}^+_{-k\downarrow} \gg = \delta_{kk'} + \ll [\hat{a}^+_{k\uparrow}, H], \hat{a}^+_{-k\downarrow} \gg$$

$$\omega \ll \hat{a}^+_{k\uparrow,}\hat{a}^+_{-k\downarrow} \gg = \ll [\hat{a}^+_{k\uparrow}, H], \hat{a}^+_{-k\downarrow} \gg. \qquad (3.2.2)$$

Solving the commutator in eq. (3.2.2) by using the Hamiltonian in eq. (3.2.1), we get

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

$$= \textstyle\sum_{p\sigma}\epsilon_p\left(\{\hat{a}^+_{k\uparrow}, \hat{a}^+_{p\uparrow}\}\hat{a}_{p\uparrow} - \hat{a}^+_{p\uparrow}\{\hat{a}^+_{k\uparrow}\hat{a}_{p\uparrow}\}\right)$$

$$= -\epsilon_k\ \hat{a}^+_{k\uparrow}, \qquad (3.2.3)$$

$$[\hat{a}^+_{k\uparrow}, M\sum_p\left(\hat{a}^+_{p+q\uparrow}\hat{a}_{p\downarrow} + \hat{a}^+_{p\downarrow}\hat{a}_{p+q\uparrow}\right)] = M\sum_p([\ \hat{a}^+_{k\uparrow}, \hat{a}^+_{p+q\uparrow}\hat{a}_{p\downarrow}] + [\hat{a}^+_{k\uparrow}, \hat{a}^+_{p\downarrow}\hat{a}_{p+q\uparrow})$$

$$= M\sum_p\left(\{\hat{a}^+_{k\uparrow}, \hat{a}^+_{p+q\uparrow}\}\hat{a}_{p\downarrow} - \hat{a}^+_{p+q\uparrow}\{\hat{a}^+_{k\uparrow}, \hat{a}_{p\downarrow}\} + \{\hat{a}^+_{k\uparrow}, \hat{a}^+_{p\downarrow}\}\hat{a}_{p+q} - \hat{a}^+_{p\downarrow}\{\hat{a}^+_{k\uparrow}, \hat{a}_{p+q\uparrow}\}\right)$$

$$= -M\hat{a}^+_{k-q\downarrow}, \qquad (3.2.4)$$

$$[\ \hat{a}^+_{k\uparrow}, \Delta_{sc}\sum_p\left(\hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right)\ ] = \Delta_{sc}\sum_p[\hat{a}^+_{k\uparrow}, \hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow}] + [\ \hat{a}^+_{k\uparrow}, \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}]$$

$$= \Delta_{sc} \sum_p \left(\{\hat{a}_{k\uparrow}^{+} \hat{a}_{p\uparrow}^{+}\} \hat{a}_{-p\downarrow}^{+} - \hat{a}_{p\uparrow}^{+} \{\hat{a}_{k\uparrow}^{+}, \hat{a}_{-p\downarrow}^{+}\} + \{\hat{a}_{k\uparrow}^{+}, \hat{a}_{-p\downarrow}\} \hat{a}_{p\uparrow} - \hat{a}_{-p\downarrow} \{\hat{a}_{k\uparrow}^{+}, \} \hat{a}_{p\uparrow} \right)$$

$$= -\Delta_{sc} \hat{a}_{-k\downarrow}, \tag{3.2.5}$$

substituting eq. (3.2.3) - eq. (3.2.5) in to eq. (3.2.2), we obtain

$$\omega \ll \hat{a}_{k\uparrow,}^{+} \hat{a}_{-k\downarrow}^{+} \gg = -\epsilon_k \ll \hat{a}_{k\uparrow,}^{+} \hat{a}_{-k\downarrow}^{+} \gg -M \ll \hat{a}_{k-q\downarrow,}^{+} \hat{a}_{-k\downarrow}^{+} \gg -\Delta_{sc} \ll \hat{a}_{-k\downarrow} \hat{a}_{-k\downarrow}^{+} \gg$$

$$(\omega + \epsilon_k) \ll \hat{a}_{k\uparrow,}^{+} \hat{a}_{-k\downarrow}^{+} \gg = -M \ll \hat{a}_{k-q\downarrow,}^{+} \hat{a}_{-k\downarrow}^{+} \gg -\Delta_{sc} \ll \hat{a}_{-k\downarrow} \hat{a}_{-k\downarrow}^{+} \gg . \tag{3.2.6}$$

The equation of motion for the correlation $\ll \hat{a}_{k-q\downarrow,}^{+} \hat{a}_{-k\downarrow}^{+} \gg$ in eq. (3.2.6) can be described as

$$\omega \ll \hat{a}_{k-q\downarrow,}^{+} \hat{a}_{-k\downarrow}^{+} \gg = \delta_{kk'} + \ll [\hat{a}_{k-q\downarrow,}^{+} H], \hat{a}_{-k\downarrow}^{+} \gg$$

$$\omega \ll \hat{a}_{k-q\downarrow,}^{+} \hat{a}_{-k\downarrow}^{+} \gg = \ll [\hat{a}_{k-q\downarrow,}^{+} H], \hat{a}_{-k\downarrow}^{+} \gg \tag{3.2.7}$$

Evaluating the commutator in eq. (3.2.7) using the Hamiltonian, we obtain

$$\left[\hat{a}_{k-q\downarrow,}^{+} \sum_{p\sigma} \epsilon_p \, \hat{a}_{p\sigma}^{+} \hat{a}_{p\sigma} \right] = \epsilon_p \sum_{p\sigma} [\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{p\sigma}^{+} \hat{a}_{p\sigma}]$$

$$= \epsilon_p \sum_p \left(\{\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{p\uparrow}^{+}\} \hat{a}_{p\uparrow} - \hat{a}_{p\uparrow}^{+} \{\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{p\uparrow}\} \right)$$

$$= -\epsilon_{k-q} \hat{a}_{k-q\downarrow}^{+}, \tag{3.2.8}$$

$$\left[\hat{a}_{k-q\downarrow,}^{+} M \sum_p \left(\hat{a}_{p+q\uparrow}^{+} \hat{a}_{p\downarrow} + \hat{a}_{p\downarrow}^{+} \hat{a}_{p+q} \right) \right] = M \sum_p \left([\hat{a}_{k-q\downarrow,}^{+} \ \hat{a}_{p+q\uparrow}^{+} \hat{a}_{p\downarrow}] + [\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{p\downarrow}^{+} \hat{a}_{p+q}] \right)$$

$$= M \sum_p \left(\{\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{p+q\uparrow}^{+}\} \hat{a}_{p\downarrow} - \hat{a}_{p+q\uparrow}^{+} \{\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{p\downarrow}\} + \{\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{p\downarrow}^{+}\} \hat{a}_{p+q} - \hat{a}_{p\downarrow}^{+} \{\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{p+q}\} \right)$$

$$= -M \hat{a}_{k\uparrow,}^{+} \tag{3.2.9}$$

$$[\hat{a}_{k-q\downarrow,}^{+} \Delta_{sc} \sum_p \left(\hat{a}_{p\uparrow}^{+} \hat{a}_{-p\downarrow}^{+} + \hat{a}_{-p\downarrow} \hat{a}_{p\uparrow} \right)] = \Delta_{sc} \sum_p \left([\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{p\uparrow}^{+} \hat{a}_{-p\downarrow}^{+}] + [\hat{a}_{k-q\downarrow,}^{+} \hat{a}_{-p\downarrow} \hat{a}_{p\uparrow}] \right)$$

$$= \Delta_{sc} \sum_p \left(0 + \{\hat{a}_{k-q\downarrow}^{+} \hat{a}_{-p\downarrow}\} \right) \hat{a}_{p\uparrow} - \hat{a}_{-p\downarrow} \{\hat{a}_{k-q\downarrow,}^{+}, \hat{a}_{p\uparrow}\}$$

$$= \Delta_{sc} \hat{a}_{-k+q\uparrow,} \tag{3.2.10}$$

substituting eq. (3.2.8) – eq. (3.2.10) into eq. (3.2.7), we get

$$\omega \ll \hat{a}_{k-q\downarrow}^{+} \hat{a}_{-k\downarrow}^{+} \gg = -\epsilon_{k-q} \ll \hat{a}_{k-q\downarrow}^{+} \hat{a}_{-k\downarrow}^{+} \gg -M \ll \hat{a}_{k\uparrow}^{+} \hat{a}_{-k\downarrow}^{+} \gg +\Delta_{sc} \ll \hat{a}_{-k+q\uparrow}, \hat{a}_{-k\downarrow}^{+} \gg$$

$$(\omega + \epsilon_{k-q}) \ll \hat{a}_{k-q\downarrow}^{+} \hat{a}_{-k\downarrow}^{+} \gg = -M \ll \hat{a}_{k\uparrow}^{+} \hat{a}_{-k\downarrow}^{+} \gg +\Delta_{sc} \ll \hat{a}_{-k+q\uparrow}, \hat{a}_{-k\downarrow}^{+} \gg . \tag{3.2.11}$$

The equation of motion for the correlation $\ll \hat{a}_{-k+q\uparrow}, \hat{a}^{+}_{-k\downarrow} \gg$ in eq. (3.2.11) is given by

$$\omega \ll \hat{a}_{-k+q\uparrow}, \hat{a}^{+}_{-k\downarrow} \gg \; = \delta_{kk'} + \ll \left[\hat{a}_{-k+q\uparrow}, H\right], \hat{a}^{+}_{-k\downarrow} \gg$$
$$= \ll \left[\hat{a}_{-k+q\uparrow}, H\right], \hat{a}^{+}_{-k\downarrow} \gg. \qquad (3.2.12)$$

Solving the commutator in eq. (3.2.12) using the Hamiltonian, we get

$$\left[\hat{a}_{-k+q\uparrow} \sum_{,p\sigma} \epsilon_p \, \hat{a}^{+}_{p\sigma}\hat{a}_{p\sigma}\right] = \sum_{p\sigma} \epsilon_p [\, \hat{a}_{-k+q\uparrow}, \; \hat{a}^{+}_{p\sigma}\hat{a}_{p\sigma}]$$
$$= \sum_{p} \epsilon_p \left(\left\{\hat{a}_{-k+q\uparrow}, \; \hat{a}^{+}_{p\sigma}\right\}\hat{a}_{p\sigma} - \hat{a}_{p\sigma}\left\{\hat{a}_{-k+q\uparrow}\hat{a}_{p\sigma}\right\}\right)$$
$$= \epsilon_{-k+q} \;\; \hat{a}_{-k+q\uparrow,} \qquad (3.2.13)$$

$$\left[\hat{a}_{-k+q\uparrow}, M \sum_{p} \left(\hat{a}^{+}_{p+q\uparrow}\hat{a}_{p\downarrow} + \; \hat{a}^{+}_{p\downarrow}\hat{a}_{p+q\uparrow}\right)\right] = M \sum_{p} \left(\left[\hat{a}_{-k+q\uparrow} \;\; \hat{a}^{+}_{p+q\uparrow}\hat{a}_{p\downarrow}\right] + [\hat{a}_{-k+q\uparrow} \; \hat{a}_{p\downarrow}\hat{a}_{p+q} \,]\right)$$
$$= M \sum_{p} \left(\left\{\hat{a}_{-k+q\uparrow} \; \hat{a}^{+}_{p+q\uparrow}\right\}\hat{a}_{p\downarrow} - \hat{a}^{+}_{p+q\uparrow}\left\{\hat{a}_{-k+q\uparrow}\hat{a}_{p\downarrow}\right\}\right)$$
$$= M\hat{a}_{-k\downarrow,} \qquad (3.2.14)$$

$$\left[\hat{a}_{-k+q\uparrow} \,, \Delta_{sc} \sum_{p} \left(\hat{a}^{+}_{p\uparrow}\hat{a}^{+}_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right)\right] = \; \Delta_{sc} \sum_{p} \left(\left[\, \hat{a}_{-k+q\uparrow}, \hat{a}^{+}_{p\uparrow}\hat{a}^{+}_{-p\downarrow} \,\right] + [\hat{a}_{-k+q\uparrow} \; \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}]\right)$$
$$= \; \Delta_{sc} \sum_{p} \left(\left\{\hat{a}_{-k+q\uparrow}, \hat{a}^{+}_{p\uparrow}\right\}\hat{a}^{+}_{-p\downarrow} - \hat{a}^{+}_{p\uparrow}\left\{\hat{a}_{-k+q\uparrow}\hat{a}^{+}_{-p\downarrow}\right\} + 0\right)$$
$$= \; \Delta_{sc}\hat{a}^{+}_{k-q\downarrow}, \qquad (3.2.15)$$

inserting eq. (3.2.13) - eq. (3.2.15) into eq. (3.2.12), we get

$$\omega \ll \hat{a}_{-k+q\uparrow}, \hat{a}^{+}_{-k\downarrow} \gg = \; \epsilon_{-k+q} \;\; \ll \hat{a}_{-k+q\uparrow}\hat{a}^{+}_{-k\downarrow} \gg \; +M \; \ll \hat{a}_{-k\downarrow}\hat{a}^{+}_{-k\downarrow} \gg + \, \Delta_{sc} \ll \hat{a}^{+}_{k-q\downarrow}\hat{a}^{+}_{-k\downarrow} \gg$$

$$\left(\omega - \epsilon_{-k+q}\,\right) \ll \hat{a}_{-k+q\uparrow}, \hat{a}^{+}_{-k\downarrow} \gg = \;\; M \; \ll \hat{a}_{-k\downarrow}\hat{a}^{+}_{-k\downarrow} \gg + \, \Delta_{sc} \ll \hat{a}^{+}_{k-q\downarrow}\hat{a}^{+}_{-k\downarrow} \gg. \qquad (3.2.16)$$

The equation of motion for the correlation $\ll \hat{a}_{-k\downarrow}\hat{a}^{+}_{-k\downarrow} \gg$ in eq. (3.2.16) is given by

$$\omega \ll \hat{a}_{-k\downarrow}\hat{a}^{+}_{-k\downarrow} \gg = \delta_{kk'} + \ll [\hat{a}_{-k\downarrow}, H], \hat{a}^{+}_{-k\downarrow} \gg$$
$$= 1 + \ll [\hat{a}_{-k\downarrow}, H], \hat{a}^{+}_{-k\downarrow} \gg. \qquad (3.2.17)$$

Evaluating the commutator in eq. (3.2.17) using eq. (3.2.1), we obtain

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

$$= \sum_{\mathrm{p}}\epsilon_{\mathrm{p}}\left(\{\hat{a}_{-k\downarrow},\hat{a}^+_{p\uparrow}\}\hat{a}_{p\uparrow} - \hat{a}^+_{p\uparrow}\{\hat{a}_{-k\downarrow}\hat{a}_{p\uparrow}\}\right)$$

$$= \epsilon_{-k}\hat{a}_{-k\downarrow,} \tag{3.2.18}$$

$$[\hat{a}_{-k\downarrow,}M\sum_p\left(\hat{a}^+_{p+q\uparrow}\hat{a}_{p\downarrow} + \hat{a}^+_{p\downarrow}\hat{a}_{p+q}\right)] = M\sum_p\left(\left[\hat{a}_{-k\downarrow,}\hat{a}^+_{p+q\uparrow}\hat{a}_{p\downarrow}\right] + [\hat{a}_{-k\downarrow},\hat{a}^+_{p\downarrow}\hat{a}_{p+q}]\right)$$

$$= M\sum_p\left(\{\hat{a}_{-k\downarrow}\hat{a}^+_{p+q\uparrow}\}\,\hat{a}_{p\downarrow} - \hat{a}^+_{p+q\uparrow}\{\hat{a}_{-k\downarrow}\hat{a}_{p\downarrow}\} + \{\hat{a}_{-k\downarrow}\hat{a}^+_{p\downarrow}\}\hat{a}_{p+q} - \hat{a}^+_{p\downarrow}\{\hat{a}_{-k\downarrow}\hat{a}_{p+q}\}\right)$$

$$= M\hat{a}_{-k+q\downarrow,} \tag{3.2.19}$$

$$[\,\hat{a}_{-k\downarrow,}\Delta_{sc}\sum_p\left(\hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right)] = \Delta_{sc}\sum_p\left([\hat{a}_{-k\downarrow},\hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow}] + [\hat{a}_{-k\downarrow},\hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}]\right)$$

$$= \Delta_{sc}\left(\{\hat{a}_{-k\downarrow},\hat{a}^+_{p\uparrow}\}\hat{a}^+_{-p\downarrow} - \hat{a}^+_{p\uparrow}\{\hat{a}_{-k\downarrow}\hat{a}^+_{-p\downarrow}\} + 0\right)$$

$$= -\Delta_{sc}\hat{a}^+_{k\uparrow,} \tag{3.2.20}$$

substituting eq. (3.2.18) - eq. (3.1.20) into eq. (3.2.17), we obtain

$$(\omega - \epsilon_{-k}) \ll \hat{a}_{-k\downarrow}\hat{a}^+_{-k\downarrow} \gg = 1 + M \ll \hat{a}_{-k+q\downarrow}\hat{a}^+_{-k\downarrow} \gg -\Delta_{sc} \ll \hat{a}^+_{k\uparrow},\hat{a}^+_{-k\downarrow} \gg. \tag{3.2.21}$$

From eq. (3.2.11), we obtain

$$\ll \hat{a}^+_{k-q\downarrow}\hat{a}^+_{-k\downarrow} \gg \;=\; \frac{-M \ll \hat{a}^+_{k\uparrow}\hat{a}^+_{-k\downarrow} \gg}{\omega+\epsilon_{k-q}} + \frac{\Delta_{sc} \ll \hat{a}_{-k+q\uparrow},\hat{a}^+_{-k\downarrow} \gg}{\omega+\epsilon_{k-q}}. \tag{3.2.22}$$

From eq. (3.2.21), we obtain

$$\ll \hat{a}_{-k\downarrow}\hat{a}^+_{-k\downarrow} \gg = \frac{1}{\omega - \epsilon_{-k}} + \frac{M \ll \hat{a}_{-k+q\downarrow}\hat{a}^+_{-k\downarrow} \gg}{\omega - \epsilon_{-k}} - \frac{\Delta_{sc} \ll \hat{a}^+_{k\uparrow},\hat{a}^+_{-k\downarrow} \gg}{\omega - \epsilon_{-k}}. \tag{3.2.23}$$

Substituting eq. (3.2.22) and eq. (3.2.23) into eq. (3.2.6), we get

$$\left((\omega + \epsilon_k) - \frac{M^2}{\omega+\epsilon_{k-q}} - \frac{\Delta^2_{sc}}{\omega - \epsilon_{-k}}\right) \ll \hat{a}^+_{k\uparrow},\hat{a}^+_{-k\downarrow} \gg = -\frac{\Delta_{sc}}{\omega - \epsilon_{-k}} -$$

$$\left(\frac{M\Delta_{sc}}{\omega+\epsilon_{k-q}} + \frac{M\Delta_{sc}}{\omega - \epsilon_{-k}}\right) \ll \hat{a}_{-k+q\uparrow},\hat{a}^+_{-k\downarrow} \gg. \tag{3.2.24}$$

Inserting eq. (3.2.22) and eq. (3.2.23) into eq. (3.2.16), we get

$$\left((\omega-\epsilon_{-k+q})-\frac{M^2}{\omega-\epsilon_{-k}}-\frac{\Delta_{sc}^2}{\omega+\epsilon_{k-q}}\right)\ll \hat{a}_{-k\downarrow},\hat{a}_{-k\downarrow}^{+}\gg=-\frac{M}{\omega-\epsilon_{-k}}-\left(\frac{M\Delta_{sc}}{\omega-\epsilon_{-k}}+\frac{M\Delta_{sc}}{\omega+\epsilon_{k-q}}\right)\ll \hat{a}_{k\uparrow}^{+},\hat{a}_{-k\downarrow}^{+}\gg . \quad (3.2.25)$$

Appling nesting condition, $\epsilon_k=-\epsilon_{k\pm q}, \epsilon_{-k}=\epsilon_{-k\mp q}$ and use approximation, $\epsilon_k=\epsilon_{-k}$, eq. (3.2.24) and eq. (3.1.25) respectively become

$$\left((\omega+\epsilon_k)-\frac{M^2}{\omega-\epsilon_k}-\frac{\Delta_{sc}^2}{\omega-\epsilon_k}\right)\ll \hat{a}_{k\uparrow}^{+},\hat{a}_{-k\downarrow}^{+}\gg=-\frac{\Delta_{sc}}{\omega-\epsilon_k}-\left(\frac{M\Delta_{sc}}{\omega-\epsilon_k}+\frac{M\Delta_{sc}}{\omega-\epsilon_k}\right)\ll \hat{a}_{-k+q\uparrow},\hat{a}_{-k\downarrow}^{+}\gg \quad (3.2.26)$$

and

$$\left((\omega+\epsilon_k)-\frac{M^2}{\omega-\epsilon_k}-\frac{\Delta_{sc}^2}{\omega-\epsilon_k}\right)\ll \hat{a}_{-k\downarrow},\hat{a}_{-k\downarrow}^{+}\gg=-\frac{M}{\omega-\epsilon_k}-\left(\frac{M\Delta_{sc}}{\omega-\epsilon_k}+\frac{M\Delta_{sc}}{\omega-\epsilon_k}\right)\ll \hat{a}_{k\uparrow}^{+},\hat{a}_{-k\downarrow}^{+}\gg . \quad (3.2.27)$$

Let x= $\omega+\epsilon_k$ and y= $\omega-\epsilon_k$

Then eq. (3.2.26) and eq. (3.2.27) respectively become

$$[\mathrm{xy}-M^2-\Delta_{sc}^2]\ll \hat{a}_{k\uparrow}^{+},\hat{a}_{-k\downarrow}^{+}\gg=-\Delta_{sc}-2M\Delta_{sc}\ll \hat{a}_{-k+q\uparrow},\hat{a}_{-k\downarrow}^{+}\gg \quad (3.2.28)$$

and

$$[\mathrm{xy}-M^2-\Delta_{sc}^2]\ll \hat{a}_{-k+q\uparrow},\hat{a}_{-k\downarrow}^{+}\gg=M-2M\Delta_{sc}\ll \hat{a}_{k\uparrow}^{+},\hat{a}_{-k\downarrow}^{+}\gg . \quad (3.2.29)$$

Derive for the correlation function $\ll \hat{a}_{-k+q\uparrow},\hat{a}_{-k\downarrow}^{+}\gg$ from eq. (3.2.29) and substituting in eq. (3.2.28), we get

$$\ll \hat{a}_{k\uparrow}^{+},\hat{a}_{-k\downarrow}^{+}\gg=\frac{-\Delta_{sc}[\mathrm{xy}-M^2-\Delta_{sc}^2+2M^2]}{[(\mathrm{xy}-M^2-\Delta_{sc}^2)^2]-[2M\Delta_{sc}]^2}$$

$$=\frac{-\Delta_{sc}[\omega^2-{\epsilon_k}^2+M^2-\Delta_{sc}^2]}{[(\omega^2-{\epsilon_k}^2-M^2-\Delta_{sc}^2)^2]-[2M\Delta_{sc}]^2} . \quad (3.2.30)$$

After some rearrangement eq. (3.2.30) can be expressed as

$$\ll \hat{a}_{k\uparrow}^{+},\hat{a}_{-k\downarrow}^{+}\gg=\frac{-1/2(\Delta_{sc}+M)}{\omega^2-\epsilon_k^2-(\Delta_{sc}+M)^2}+\frac{-1/2(\Delta_{sc}-M)}{\omega^2-\epsilon_k^2-(\Delta_{sc}-M)^2} . \quad (3.2.31)$$

Using the expression $\omega \to i\omega_n$, we obtain

$$\ll \quad \hat{a}^{+}_{k\uparrow}, \hat{a}^{+}_{-k\downarrow} \gg = \frac{1/2(\Delta_{sc}+M)}{\omega_n^2+\epsilon_k^2+(\Delta_{sc}+M)^2} + \frac{1/2(\Delta_{sc}-M)}{\omega_n^2+\epsilon_k^2+(\Delta_{sc}-M)^2}, \qquad (3.2.32)$$

we express $\Delta_j(k) = \Delta_{sc} - (-1)^j M$,where $\Delta_j(k)$ is effective order parameter,

$$\ll \hat{a}^{+}_{k\uparrow}, \hat{a}^{+}_{-k\downarrow} \gg \; = \frac{1/2\Delta_j(k)}{\omega_n^2+\epsilon_k^2+\Delta_j^2(k)} + \frac{1/2\Delta_j(k)}{\omega_n^2+\epsilon_k^2+\Delta_j^2(k)} \qquad (3.3.33)$$

$$\ll \hat{a}^{+}_{k\uparrow}, \hat{a}^{+}_{-k\downarrow} \gg \; = \frac{1}{2}\sum_{j=1,2} \frac{\Delta_j(k)}{\omega_n^2+\epsilon_k^2+\Delta_j^2(k)}. \qquad (3.2.34)$$

From Matsubara's frequency, we have

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

Substituting the above relation into eq. (3.2.34), we get

$$\ll \hat{a}^{+}_{k\uparrow}, \hat{a}^{+}_{-k\downarrow} \gg = \frac{1}{2}\sum_{j=1,2} \frac{\beta^2\Delta_j(k)}{(2n+1)^2\pi^2+\beta^2(\epsilon_k^2+\Delta_j^2(k))}. \qquad (3.2.35)$$

The superconductivity order parameter Δ_{sc} is given by

$$\Delta_{sc} = \frac{V}{\beta}\sum_{k,n} \ll \hat{a}^{+}_{k\uparrow}, \hat{a}^{+}_{-k\downarrow} \gg. \qquad (3.2.36)$$

Insert eq. (3.2.35) into eq. (3.2.36), we obtain

$$\Delta_{sc} = \frac{V}{2}\sum_{k,nj=1,2} \frac{\beta\Delta_j(k)}{(2n+1)^2\pi^2+\beta^2(\epsilon_k^2+\Delta_j^2(k))}. \qquad (3.2.37)$$

Let us represent $\gamma = \beta(\epsilon_k^2+\Delta_j^2(k))^{\frac{1}{2}}$ (3.2.38)

and

$$\sum_{-\infty}^{\infty} \frac{1}{(2n+1)^2\pi^2+\gamma^2} = \frac{\tanh\gamma/2}{2\gamma}. \qquad (3.2.39)$$

Substituting eq. (3.2.38) and eq. (3.2.39) into eq. (3.2.37), we obtain

$$\Delta_{sc} = \frac{\mathrm{V}}{4}\sum_{\mathrm{k,j=1,2}} \frac{\Delta_j(k)\tanh\frac{\beta}{2}(\epsilon_k^2+\Delta_j^2(k))^{\frac{1}{2}}}{(\epsilon_k^2+\Delta_j^2(k))^{\frac{1}{2}}}. \qquad (3.2.40)$$

Converting the summation over k values into an integral with the cut-off energy from $\pm\hbar\omega_b$ measured from the Fermi level and use the density of state at the Fermi level is N (o).

The density of state N (o) is equal to $N(o)_1+N(o)_2$. Assume $N(o)_1=N(o)_2$ this implies that $N(o)_2=N(o)/2$. So for j=2

$$\Delta_{sc}=\frac{N(O)_2\,V}{2}\int_{-\hbar\omega_b}^{\hbar\omega_b}\frac{(\Delta_{sc}-M)\tanh\frac{\beta}{2}(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}{(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}\,d\epsilon_k \tag{3.2.41}$$

$\lambda = N(O)_2\,V$, and eq. (3.2.41) becomes

$$\Delta_{sc}=\lambda\int_0^{\hbar\omega_b}(\Delta_{sc}-M)\,\frac{\tanh\frac{\beta}{2}(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}{(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}\,d\epsilon_k. \tag{3.2.42}$$

Divided the above equation by Δ_{sc} we have,

$$\frac{1}{\lambda}=\int_0^{\hbar\omega_b}\left(1-\frac{M}{\Delta_{sc}}\right)\frac{\tanh\frac{\beta}{2}(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}{(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}\,d\epsilon_k. \tag{3.2.43}$$

Let us study eq. (3.2.43) for different cases

Case I when $T\rightarrow 0, \beta\rightarrow\infty$, which implies,

$\tanh\frac{\beta}{2}(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}} \rightarrow 1$. Eq. (3.2.43) becomes,

$$\frac{1}{\lambda}=\int_0^{\hbar\omega_b}\frac{\left(1-\frac{M}{\Delta_{sc}}\right)}{(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}\,d\epsilon_k. \tag{3.2.44}$$

Using the integral relation below

$$\int\frac{y}{\sqrt{y^2+x^2}}\,dx = y\sinh^{-1}(x/y),$$

eq. (3.2.44) evaluated as

$$\frac{1}{\lambda}=\left(1-\frac{M}{\Delta_{sc}}\right)\sinh^{-1}\frac{(\hbar\omega_b)}{(\Delta_{sc}-M)} \tag{3.2.45}$$

$$\frac{1}{\lambda}=\left(1-\frac{M}{\Delta_{sc}}\right)\ln\left\{\frac{\hbar\omega_b}{\Delta_{sc}-M}+\sqrt{\left(\frac{\hbar\omega_b}{\Delta_{sc}-M}\right)^2+1}\right\}$$

$$\frac{\Delta_{sc}}{\lambda}=(\Delta_{sc}-M)\ln\left\{\frac{\hbar\omega_b}{\Delta_{sc}-M}+\sqrt{\left(\frac{\hbar\omega_b}{\Delta_{sc}-M}\right)^2+1}\right\}$$

$$\frac{\Delta_{sc}}{\lambda} \approx (\Delta_{sc} - M) \ln \frac{2\hbar\omega_b}{\Delta_{sc} - M}$$

$$exp\left(\frac{\Delta_{sc}}{\lambda(\Delta_{sc} - M)}\right) = \frac{2\hbar\omega_b}{\Delta_{sc} - M}$$

$$\Delta_{sc} - M = 2\hbar\omega_b \exp\left(-\frac{1}{\lambda\left(1 - \frac{M}{\Delta_{sc}}\right)}\right). \quad (3.2.46)$$

If the magnetic order parameter is zero eq. (3.2.46) becomes

$$\Delta_{sc} = 2\hbar\omega_b \exp\left(-\frac{1}{\lambda}\right). \quad (3.2.47)$$

When T→ 0, Δ_{sc}→ $\Delta_{sc}(0)$, the BCS theory expressed as

$$\frac{2\Delta_{sc}(0)}{k_\beta T_c} = 3.5$$

Using the above expression, eq. (3.2.47) becomes

$$k_\beta T_c = 1.14\, \hbar\omega_b \exp\left(-\frac{1}{\lambda}\right). \quad (3.2.48)$$

Eq. (3.2.48) is the BCS expression for superconducting transition temperature (T_c).

$$\text{From } \frac{2\Delta_{sc}(0)}{k_\beta T_c} = 3.5$$

we have

$$\Delta_{sc}(0) = 1.75 k_\beta T_c.$$

Substituting the above expression into eq. (3.2.46), we obtain

$$M = 1.75 k_\beta T_c - 2\hbar\omega_b \exp\left(-\frac{1}{\lambda\left(1 - \frac{M}{1.75 k_\beta T_c}\right)}\right). \quad (3.2.46.1)$$

To solve this equation numerically we use Debay temperature equal to 315.7K [37,38] and the interband BCS coupling constant is 0.5[39].

Case II as T→ T_c, Δ_{sc}→ 0

Eq. (3.2.43) can be written as;

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}(\epsilon_k^2 + (\Delta_{sc} - M)^2)^{\frac{1}{2}}}{(\epsilon_k^2 + (\Delta_{sc} - M)^2)^{\frac{1}{2}}}\, d\epsilon_k - \int_0^{\hbar\omega_b} \frac{M}{\Delta_{sc}} \frac{\tanh\frac{\beta}{2}(\epsilon_k^2 + (\Delta_{sc} - M)^2)^{\frac{1}{2}}}{(\epsilon_k^2 + (\Delta_{sc} - M)^2)^{\frac{1}{2}}}\, d\,\epsilon_k.$$

(3.2.49)

In order to calculate the first integral of the RHS of eq. (3.2.49) for $\Delta_{sc} = 0$,

let $\gamma = \beta\sqrt{\epsilon_k^2 + M^2}$.

Thus, the first integral in the RHS of eq. (3.2.49) can be write as,

$$\int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}(\epsilon_k^2 + M^2)^{\frac{1}{2}}}{(\epsilon_k^2 + M^2)^{\frac{1}{2}}}\, d\epsilon_k = \int_0^{\hbar\omega_b} \frac{2\beta\tanh\frac{\gamma}{2}}{2\gamma}. \qquad (3.2.50)$$

Applying the equality below and inserting it in eq. (3.2.50), we get

$$\sum_{-\infty}^{\infty} \frac{1}{(2n+1)^2\pi^2 + \gamma^2} = \frac{\tanh\gamma/2}{2\gamma}$$

$$\int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}(\epsilon_k^2 + M^2)^{\frac{1}{2}}}{(\epsilon_k^2 + M^2)^{\frac{1}{2}}}\, d\epsilon_k = \int_0^{\hbar\omega_b} 2\beta \sum_{-\infty}^{\infty} \frac{1}{(2n+1)^2\pi^2 + \gamma^2}\, d\epsilon_k. \qquad (3.2.51)$$

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

Using the above relation and simplifying eq. (3.2.51), we get

$$\int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}(\epsilon_k^2 + M^2)^{\frac{1}{2}}}{(\epsilon_k^2 + M^2)^{\frac{1}{2}}}\, d\epsilon_k = \int_0^{\hbar\omega_b} \frac{2}{\beta} \sum_{-\infty}^{\infty} \frac{1}{\omega_n^2 + \epsilon_k^2 + M^2}\, d\epsilon_k. \qquad (3.2.52)$$

Using Laplacian's Transformation together with Matsuber relation eq. (3.2.52) becomes

$$\int_0^{\hbar\omega_b} \frac{2}{\beta} \sum_{-\infty}^{\infty} \frac{1}{\omega_n^2 + \epsilon_k^2 + M^2}\, d\epsilon_k = \int_0^{\hbar\omega_b} \frac{2}{\beta} \sum_{-\infty}^{\infty} \frac{1}{\omega_n^2 + \epsilon_k^2}\, d\epsilon_k -$$

$$M^2 \int_0^{\hbar\omega_b} \frac{2}{\beta} \sum_{-\infty}^{\infty} \frac{1}{(\omega_n^2 + \epsilon_k^2)^2}\, d\epsilon_k. \qquad (3.2.53)$$

The first integral of the RHS of eq. (3.2.53) is evaluated as

$$\int_0^{\hbar\omega_b} \frac{2}{\beta} \sum_{-\infty}^{\infty} \frac{1}{\omega_n^2 + \epsilon_k^2}\, d\epsilon_k = \int_0^{\hbar\omega_b} 2\beta \sum_{-\infty}^{\infty} \frac{1}{(2n+1)^2\pi^2 + (\beta\epsilon_k)^2}\, d\epsilon_k$$

$$\int_0^{\hbar\omega_b} \frac{2}{\beta}\sum_{-\infty}^{\infty}\frac{1}{\omega_n^2+\epsilon_k^2}d\epsilon_k \quad = \int_0^{\hbar\omega_b}\frac{\tanh\beta\epsilon_k/2}{\epsilon_k}\ d\epsilon_k. \qquad (3.2.53.1)$$

The second integral of the RHS of eq. (3.2.53) can be evaluated as

$$M^2\int_0^{\hbar\omega_b}\frac{2}{\beta}\sum_{-\infty}^{\infty}\frac{1}{(\omega_n^2+\epsilon_k^2)^2}d\epsilon_k = \quad M^2\int_0^{\hbar\omega_b}\frac{2}{\beta}\sum_{-\infty}^{\infty}\frac{1}{\left((2n+1)^2(\frac{\pi}{\beta})^2+\epsilon_k^2\right)^2}d\epsilon_k$$

$$= 2M^2\int_0^{\hbar\omega_b}\frac{2}{\beta}\sum_{n=0}^{\infty}\frac{1}{\left((2n+1)^2(\frac{\pi}{\beta})^2+\epsilon_k^2\right)^2}d\epsilon_k.$$

Using the following equality

$$2\sum_{n=0}^{\infty}\frac{1}{(a^2+\epsilon_k^2)^2} = 2\sum_{n=0}^{\infty}\frac{1}{(a^4(1+x^2)^2},$$

where $x^2=\frac{\epsilon_k^2}{a^2}$ and a= $(2n+1)\frac{\pi}{\beta}$

eq. (3.2.52) is equal to

$$\int_0^{\hbar\omega_b}\frac{\tanh\frac{\beta}{2}(\epsilon_k^2+M^2)^{\frac{1}{2}}}{(\epsilon_k^2+M^2)^{\frac{1}{2}}}\ d\epsilon_k = \int_0^{\hbar\omega_b}\frac{\tanh\beta\epsilon_k/2}{\epsilon_k}\ d\epsilon_k - \int_0^{\hbar\omega_b}\frac{4}{\beta}\sum_{n=0}^{\infty}\frac{M^2}{a^4(1+x^2)^2}. \qquad (3.2.54)$$

To evaluate the RHS eq. (3.2.54), let x=$\beta\epsilon_k/2 \rightarrow dx = {}^{\beta d\epsilon_k}/_2$ and using integral by part,

$$\int_0^{\hbar\omega_b}\frac{\tanh\beta\epsilon_k/2}{\epsilon_k}\ d\epsilon_k = \int_0^{\frac{\beta}{2}\hbar\omega_b}\frac{\tanh x}{x}\ dx$$

$$\int_0^{\hbar\omega_b}\frac{\tanh\beta\epsilon_k/2}{\epsilon_k}\ d\epsilon_k \quad = \ln x\tanh(\tfrac{\hbar\omega_b}{2k_\beta T}) - \int_0^{\frac{\beta}{2}\hbar\omega_b}\frac{\ln x}{\cos h^2 x}dx$$

for low temperature $\tanh(\frac{\hbar\omega_b}{2k_\beta T}) \rightarrow 1$,

$$\Rightarrow \int_0^{\hbar\omega_b}\frac{\tanh\beta\epsilon_k/2}{\epsilon_k}\ d\epsilon_k = \ln\frac{\beta\hbar\omega_b}{2} - \ln({}^{\pi}/_{4\gamma})$$

$$= \ln 1.14\frac{\hbar\omega_b}{k_\beta T_c}. \qquad (3.2.54.1)$$

Where γ denotes the Euler's constant and its value is given by

$$\gamma = 1.78.$$

The second integral of the RHS of eq. (3.2.54) can be evaluated as

$$\int_0^{\hbar\omega_b} \frac{4}{\beta}\sum_{n=0}^{\infty}\frac{M^2}{a^4(1+x^2)^2}\, d\epsilon_k = \quad \frac{4}{\beta}M^2\sum_{n=0}\frac{1}{a^3}\int_0^{\infty}\frac{1}{(1+x^2)^2}\, dx$$

$$= \frac{4\beta^2 M^2}{\pi^3}\sum_{n=0}\frac{1}{(2n+1)^3}\int_0^{\infty}\frac{1}{(1+x^2)^2}\, dx$$

$$= \frac{4\beta^2 M^2}{\pi^3}\frac{7}{8}\xi(3)\,{}^{\pi}\!/_4$$

$$= \left(\frac{M}{\pi k_\beta T_c}\right)^2 1.05. \qquad (3.2.54.2)$$

Where

$$\int_0^{\infty}\frac{1}{1+x^2}dx = {}^{\pi}\!/_4 \; and \sum_0^{\infty}\frac{1}{(2n+1)^p} = (1-2^{-p})\xi(p)$$

Here p=3, $\xi(p) = 1.202$ and ξ is zata function.

Therefore, the first integral of the RHS of eq. (3.2.49) is the sum of eq. (3.1.54.1) and eq. (3.2.54.2) and is given by

$$\int_0^{\hbar\omega_b}\frac{\tanh\frac{\beta}{2}(\epsilon_k^2+M^2)^{\frac{1}{2}}}{(\epsilon_k^2+M^2)^{\frac{1}{2}}}\, d\epsilon_k = \ln 1.14\frac{\hbar\omega_b}{k_\beta T_c} - M^2\left(\frac{1}{\pi k_\beta T_c}\right)^2 1.052. \qquad (3.2.55)$$

The second integral (Φ stands for the second integral) of the RHS of eq. (3.2.49) can be calculated by using L'Hopitals Rule as follows

$$\Phi \quad = -\int_0^{\hbar\omega_b}\lim_{\Delta_{sc}\to 0}\frac{d}{d\Delta_{sc}}[\left(\frac{M}{\Delta_{sc}}\right)\frac{\tanh\frac{\beta}{2}(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}{(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}]d\,\epsilon_k$$

$$\Phi \quad = -\int_0^{\hbar\omega_b}\lim_{\Delta_{sc}\to 0}[\frac{M\sec h^2\frac{\beta}{2}(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}\;\; \frac{\beta}{2}\frac{(\Delta_{sc}-M)}{(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}}{(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}} \;\; + \frac{\Delta_{sc}(\Delta_{sc}-M)}{(\epsilon_k^2+(\Delta_{sc}-M)^2)^{\frac{1}{2}}}}d\,\epsilon_k$$

$$= \int_0^{\hbar\omega_b}\frac{\beta M^2}{2}\frac{\sec h^2\frac{\beta}{2}(\epsilon_k^2+M^2)^{\frac{1}{2}}\;\;\frac{1}{(\epsilon_k^2+M^2)^{\frac{1}{2}}}}{(\epsilon_k^2+M^2)^{\frac{1}{2}}}]d\,\epsilon_k$$

$$\Phi = \int_0^{\hbar\omega_b} \frac{\beta M^2}{2} \frac{\sec h^2 \frac{\beta}{2} (\epsilon_k^2 + M^2)^{\frac{1}{2}}}{(\epsilon_k^2 + M^2)} d\,\epsilon_k.$$

Therefore, we can write eq. (3.2.49) as

$$\frac{1}{\lambda} = \ln 1.14 \tfrac{\hbar\omega_b}{k_\beta T_c} - M^2 \left(\frac{1}{\pi k_\beta T_c}\right)^2 1.052 + \int_0^{\hbar\omega_b} \frac{\beta M^2}{2} \frac{\sec h^2 \frac{\beta}{2} (\epsilon_k^2 + M^2)^{\frac{1}{2}}}{(\epsilon_k^2 + M^2)} d\epsilon_k. \qquad (3.2.49.1)$$

For pure superconductors (M= 0) , eq. (3.2.49) becomes

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} \frac{\tanh \frac{\beta}{2} (\epsilon_k^2 + \Delta_{sc}^2)^{\frac{1}{2}}}{(\epsilon_k^2 + \Delta_{sc}^2)^{\frac{1}{2}}} d\epsilon_k. \qquad (3.2.56)$$

To evaluate eq. (3.2.56), we use the same method to solve the RHS integral of eq. (3.2.49). By using this method we get,

$$\frac{1}{\lambda} = \ln 1.14 \tfrac{\hbar\omega_b}{k_\beta T} - \Delta_{sc}^2 \left(\frac{1}{\pi k_\beta Tc}\right)^2 1.05 \qquad (3.2.57)$$

From BCS theory when T→ 0,

$$k_\beta T_c = 1.14\hbar\omega_b \exp\left(\tfrac{-1}{\lambda}\right)$$

$$\Rightarrow \frac{1}{\lambda} = \ln 1.14 \tfrac{\hbar\omega_b}{k_\beta T_c}\,. \qquad (3.2.58)$$

Inserting eq. (3.2.58) into eq. (3.2.57), we get

$$\ln 1.14 \tfrac{\hbar\omega_b}{k_\beta T_c} = \ln 1.14 \tfrac{\hbar\omega_b}{k_\beta T} - \Delta_{sc}^2 \left(\frac{1}{\pi k_\beta Tc}\right)^2 1.052$$

$$\ln(T/_{T_c}) = -\Delta_{sc}^2 \left(\frac{1}{\pi k_\beta Tc}\right)^2 1.05\,2\,. \qquad (3.2.59)$$

Using logarithmic series $\ln(1-x) = -x - x^2/_2$, we obtained

$$\ln(T/_{T_c}) = (1 - \left(1 - T/_{T_c}\right) = -\left(1 - T/_{T_c}\right) - \frac{\left(1 - T/_{T_c}\right)^2}{2}$$

$$\approx -\left(1 - T/_{T_c}\right). \qquad (3.2.60)$$

Substituting eq. (3.2.60) into eq. (3.2.59), we obtain

$$-\left(1-{}^{T}/_{T_c}\right) = -\Delta_{sc}^2\left(\frac{1}{\pi k_\beta Tc}\right)^2 1.052$$

$$\Rightarrow \quad \Delta_{sc} = 3.306 k_\beta T_c \left(1-{}^{T}/_{T_c}\right)^{\frac{1}{2}}. \qquad (3.2.61)$$

Eq. (3.2.61) is superconducting order parameter as a function of temperature

3.2.2 The Order parameter of SDW

The equation of motion for the correlation $\ll \hat{a}^+_{k\uparrow,}\hat{a}_{k-q\downarrow} \gg$ to express the order parameter of SDW can be described as;

$$\omega \ll \hat{a}^+_{k\uparrow,}\hat{a}_{k-q\downarrow} \gg = \delta_{kk'} + \ll [\hat{a}^+_{k\uparrow}, H], \hat{a}_{k-q\downarrow} \gg$$

$$\omega \ll \hat{a}^+_{k\uparrow,}\hat{a}_{k-q\downarrow} \gg = \ll [\hat{a}^+_{k\uparrow}, H], \hat{a}_{k-q\downarrow} \gg. \qquad (3.2.62)$$

Evaluating the commutator in eq. (3.2.62) by using eq. (3.2.1), we obtain

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

$$= \sum_p \epsilon_p \left(\{\hat{a}^+_{k\uparrow}, \hat{a}^+_{p\uparrow}\}\hat{a}_{p\uparrow} - \hat{a}^+_{p\uparrow}\{\hat{a}^+_{k\uparrow}\hat{a}_{p\uparrow}\}\right)$$

$$= -\sum_p \epsilon_p\, \hat{a}^+_{p\uparrow}\delta_{kp}\delta_{\uparrow\uparrow}$$

$$= -\epsilon_k \hat{a}^+_{k\uparrow,} \qquad (3.2.63)$$

$$[\hat{a}^+_{p\uparrow}, M\sum_p \left(\hat{a}^+_{p+q\uparrow}\hat{a}_{p\downarrow} + \hat{a}^+_{p\downarrow}\hat{a}_{p+q\uparrow}\right)] = M\sum_p ([\hat{a}^+_{k\uparrow}, \hat{a}^+_{p+q\uparrow}\hat{a}_{p\downarrow}] + [\hat{a}^+_{k\uparrow}, \hat{a}^+_{p\downarrow}\hat{a}_{p+q\uparrow})$$

$$= M\sum_p \left(\{\hat{a}^+_{k\uparrow}, \hat{a}^+_{p+q\uparrow}\}\hat{a}_{p\downarrow} - \hat{a}^+_{p+q\uparrow}\{\hat{a}^+_{k\uparrow}, \hat{a}_{p\downarrow}\} + \{\hat{a}^+_{k\uparrow}, \hat{a}^+_{p\downarrow}\}\hat{a}_{p+q} - \hat{a}^+_{p\downarrow}\{\hat{a}^+_{k\uparrow}, \hat{a}_{p+q\uparrow}\}\right)$$

$$= -M\hat{a}_{p\downarrow}\delta_{k,p+q}\delta_{\uparrow\uparrow}$$

$$= -M\hat{a}_{k-q\downarrow,} \qquad (3.2.64)$$

$$[\hat{a}^+_{k\uparrow}, \Delta_{sc}\sum_p \left(\hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right)] = \Delta_{sc}\sum_p [\hat{a}^+_{k\uparrow}, \hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow}] + [\hat{a}^+_{k\uparrow}, \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}]$$

$$= \Delta_{sc}\sum_p \left(\{\hat{a}^+_{k\uparrow}\hat{a}^+_{p\uparrow}\}\hat{a}^+_{-p\downarrow} - \hat{a}^+_{p\uparrow}\{\hat{a}^+_{k\uparrow}, \hat{a}^+_{-p\downarrow}\} + \{\hat{a}^+_{k\uparrow}, \hat{a}_{-p\downarrow}\}\hat{a}_{p\uparrow} - \hat{a}_{-p\downarrow}\{\hat{a}^+_{k\uparrow},\}\hat{a}_{p\uparrow}\right)$$

$$= -\Delta_{sc}\hat{a}_{-p\downarrow}\delta_{kp}\delta_{\uparrow\uparrow}$$

$$= -\Delta_{sc}\hat{a}_{-k\downarrow,} \qquad (3.2.65)$$

substituting eq. (3.2.63)- eq. (3.2.65) into eq. (3.2.62), we get

$$\omega \ll \hat{a}^{+}_{k\uparrow,}\hat{a}_{k-q\downarrow} \gg = -\epsilon_k \ll \hat{a}^{+}_{k\uparrow,}\hat{a}_{k-q\downarrow} \gg -M \ll \hat{a}^{+}_{k-q\downarrow,}\hat{a}_{k-q\downarrow} \gg -\Delta_{sc} \ll \hat{a}_{-k\downarrow}\hat{a}_{k-q\downarrow} \gg$$

$$(\omega+\epsilon_k) \ll \hat{a}^{+}_{k\uparrow,}\hat{a}_{k-q\downarrow} \gg = -M \ll \hat{a}^{+}_{k-q\downarrow,}\hat{a}_{k-q\downarrow} \gg -\Delta_{sc} \ll \hat{a}_{-k\downarrow}\hat{a}_{k-q\downarrow} \gg. \qquad (3.2.66)$$

The equation of motion for the correlation $\ll \hat{a}^{+}_{k-q\downarrow,}\hat{a}_{k-q\downarrow} \gg$ in eq. (3.2.66) can be

$$\omega \ll \hat{a}^{+}_{k-q\downarrow,}\hat{a}_{k-q\downarrow} \gg = \delta_{kk'} + \ll \left[\hat{a}^{+}_{k-q\downarrow,}H\right], \hat{a}_{k-q\downarrow} \gg$$

$$\omega \ll \hat{a}^{+}_{k-q\downarrow,}\hat{a}_{k-q\downarrow} \gg = 1 + \ll \left[\hat{a}^{+}_{k-q\downarrow,}H\right], \hat{a}_{k-q\downarrow} \gg. \qquad (3.2.67)$$

Solving the commutator in eq. (3.2.67) using the Hamiltonian, we get

$$\left[\hat{a}^{+}_{k-q\downarrow,} \sum_{p\sigma} \epsilon_p \, \hat{a}^{+}_{p\sigma}\hat{a}_{p\sigma}\right] = \epsilon_p \sum_{p} [\hat{a}^{+}_{k-q\downarrow,}\hat{a}^{+}_{p\sigma}\hat{a}_{p\sigma}]$$

$$= \epsilon_p \sum_{p} \left(\{\hat{a}^{+}_{k-q\downarrow,}\hat{a}^{+}_{p\uparrow}\}\hat{a}_{p\uparrow} - \hat{a}^{+}_{p\uparrow}\{\hat{a}^{+}_{k-q\downarrow,}\hat{a}_{p\uparrow}\}\right)$$

$$= -\epsilon_{k-q}\hat{a}^{+}_{k-q\downarrow}, \qquad (3.2.68)$$

$$\left[\hat{a}^{+}_{k-q\downarrow,} M \sum_{p} \left(\hat{a}^{+}_{p+q\uparrow}\hat{a}_{p\downarrow} + \hat{a}^{+}_{p\downarrow}\hat{a}_{p+q\uparrow}\right)\right] = M \sum_{p} \left(\left[\hat{a}^{+}_{k-q\downarrow,} \; \hat{a}^{+}_{p+q\uparrow}\hat{a}_{p\downarrow}\right] + \left[\hat{a}^{+}_{k-q\downarrow,} \; \hat{a}^{+}_{p\downarrow}\hat{a}_{p+q\uparrow}\right] \right)$$

$$= M \sum_{p} \left(\{\hat{a}^{+}_{k-q\downarrow,}\hat{a}^{+}_{p+q\uparrow}\}\hat{a}_{p\downarrow} - \hat{a}^{+}_{p+q\uparrow}\{\hat{a}^{+}_{k-q\downarrow,}\hat{a}_{p\downarrow}\} + \{\hat{a}^{+}_{k-q\downarrow,}\hat{a}^{+}_{p\downarrow}\}\hat{a}_{p+q} - \hat{a}^{+}_{p\downarrow}\{\hat{a}^{+}_{k-q\downarrow,}\hat{a}_{p+q\uparrow}\}\right)$$

$$= -M\hat{a}^{+}_{k\uparrow}, \qquad (3.2.69)$$

$$[\, \hat{a}^{+}_{k-q\downarrow,} \, \Delta_{sc} \sum_{p} \left(\hat{a}^{+}_{p\uparrow}\hat{a}^{+}_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right)] = \Delta_{sc} \sum_{p} \left(\left[\, \hat{a}^{+}_{k-q\downarrow,}\hat{a}^{+}_{p\uparrow}\hat{a}^{+}_{-p\downarrow}\,\right] + [\hat{a}^{+}_{k-q\downarrow,} \; \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}]\right)$$

$$= \Delta_{sc} \sum_{p} \left(0 + \{\hat{a}^{+}_{k-q\downarrow}\hat{a}_{-p\downarrow}\}\right)\hat{a}_{p\uparrow} - \hat{a}_{-p\downarrow}\{\hat{a}^{+}_{k-q\downarrow,}, \hat{a}_{p\uparrow}\}$$

$$= \Delta_{sc}\hat{a}_{-k+q\uparrow,} \qquad (3.2.70)$$

inserting eq. (3.2.68) – eq. (3.2.70) into eq. (3.2.67), we obtain

$$\left(\omega + \epsilon_{k-q}\right) \ll \hat{a}^{+}_{k-q\downarrow,}\hat{a}_{k-q\downarrow} \gg = 1 - M \ll \hat{a}^{+}_{k\uparrow}, \hat{a}_{k-q\downarrow} \gg + \Delta_{sc} \ll \hat{a}_{-k+q\uparrow}\hat{a}_{k-q\downarrow} \gg. \quad (3.2.71)$$

The equation of motion for the correlation $\ll \hat{a}_{-+\uparrow}, \hat{a}_{k-q\downarrow} \gg$ in eq. (3.2.71) is expressed as

$$\omega \ll \hat{a}_{-k+q\uparrow}\hat{a}_{k-q\downarrow} \gg = \delta_{kk'} + \ll \left[\hat{a}_{-k+q\uparrow}H\right], \hat{a}_{k-q\downarrow} \gg$$

$$= \ll \left[\hat{a}_{-k+q\uparrow}H\right], \hat{a}_{k-q\downarrow} \gg. \qquad (3.2.72)$$

Evaluating the commutator using the Hamiltonian in eq. (3.2.1), we obtain

$$\left[\hat{a}_{-k+q\uparrow}\sum_{,p\sigma}\epsilon_p\,\hat{a}^{+}_{p\sigma}\hat{a}_{p\sigma}\right] = \sum_{,p\sigma}\epsilon_p[\,\hat{a}_{-k+q\uparrow},\ \hat{a}^{+}_{p\uparrow}\hat{a}_{p\uparrow}]$$

$$= \sum_{p}\epsilon_p\left(\{\hat{a}_{-k+q\uparrow},\ \hat{a}^{+}_{p\uparrow}\}\hat{a}_{p\uparrow} - \hat{a}_{p\sigma}\{\hat{a}_{-k+q\uparrow}\hat{a}_{p\uparrow}\}\right)$$

$$= \epsilon_{-k+q}\hat{a}_{-k+q\uparrow,} \tag{3.2.73}$$

$$\left[[\hat{a}_{-k+q\uparrow}, M\sum_{p}\left(\hat{a}^{+}_{p+q\uparrow}\hat{a}_{p\downarrow} +\ \hat{a}^{+}_{p\downarrow}\hat{a}_{p+q\uparrow}\ \right)\right] = M\sum_{p}\left(\ [\hat{a}_{-k+q\uparrow}\ \ \hat{a}^{+}_{p+q\uparrow}\hat{a}^{+}_{p\downarrow}] + [\hat{a}_{-k+q\uparrow}\ \hat{a}^{+}_{p\downarrow}\hat{a}_{p+q\uparrow}\ ]\right)$$

$$= M\sum_{p}\left(\{\hat{a}_{-k+q\uparrow}\ \hat{a}^{+}_{p+q\uparrow}\}\hat{a}^{+}_{p\downarrow} - \hat{a}^{+}_{p+q\uparrow}\{\hat{a}_{-k+q\uparrow}\hat{a}^{+}_{p\downarrow}\}\right)$$

$$= M\hat{a}_{-k\downarrow} \tag{3.2.74}$$

$$\left[\hat{a}_{-k+q\uparrow}\ ,\Delta_{sc}\sum_{p}\left(\hat{a}^{+}_{p\uparrow}\hat{a}^{+}_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right)\right] = \ \Delta_{sc}\sum_{p}\left([\ \hat{a}_{-k+q\uparrow}, \hat{a}^{+}_{p\uparrow}\hat{a}^{+}_{-p\downarrow}\ ] + [\hat{a}_{-k+q\uparrow}\ \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}]\right)$$

$$= \ \Delta_{sc}\sum_{p}\left(\{\hat{a}_{-k+q\uparrow}, \hat{a}^{+}_{p\uparrow}\}\hat{a}^{+}_{-p\downarrow} - \hat{a}^{+}_{p\uparrow}\{\hat{a}_{-k+q\uparrow}\hat{a}^{+}_{-p\downarrow}\} + 0\right)$$

$$= \ \Delta_{sc}\hat{a}^{+}_{k-q\downarrow}, \tag{3.2.75}$$

substituting eq. (3.2.73) – eq. (3.2.75) into eq. (3.2.72), we get

$$\left(\omega - \epsilon_{-k+q}\right) \ll \hat{a}_{-k+q\uparrow}\hat{a}_{k-q\downarrow} \gg = M \ll \hat{a}_{-k\downarrow,}\hat{a}_{k-q\downarrow} \gg + \Delta_{sc} \ll \hat{a}^{+}_{k-q\downarrow,}\hat{a}_{k-q\downarrow} \ \gg. \tag{3.2.76}$$

The equation of motion for the correlation $\ll \hat{a}_{-k\downarrow,}\hat{a}_{k-q\downarrow} \gg$ in eq.(3.2.76) is describ as

$$\omega \ll \hat{a}_{-k\downarrow,}\hat{a}_{k-q\downarrow} \gg = \delta_{kk'} + \ll [\hat{a}_{-k\downarrow,}H]\hat{a}_{k-q\downarrow} \gg$$

$$\omega \ll \hat{a}_{-k\downarrow,}\hat{a}_{k-q\downarrow} \gg = \ll \left[\hat{a}_{-k\downarrow,}H\right]\hat{a}_{k-q\downarrow} \gg. \tag{3.2.77}$$

The commutator in eq. (3.2.77) can be calculated as

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

$$[\ \hat{a}_{-k\downarrow,}\sum_{p\sigma}\epsilon_p\ \hat{a}^{+}_{p\sigma}\hat{a}_{p\sigma}] \quad = \sum_{\mathrm{p}}\epsilon_{\mathrm{p}}\left(\{\hat{a}_{-k\downarrow,}\hat{a}^{+}_{p\uparrow}\}\hat{a}_{p\uparrow} - \hat{a}^{+}_{p\uparrow}\{\hat{a}_{-k\downarrow}\hat{a}_{p\uparrow}\}\right)$$

$$= \epsilon_{-k}\hat{a}_{-k\downarrow,} \tag{3.2.78}$$

$$[\hat{a}_{-k\downarrow}, M\sum_p(\hat{a}^+_{p+q\uparrow}\hat{a}_{p\downarrow} + \hat{a}^+_{p\downarrow}\hat{a}_{p+q\uparrow})] = M\sum_p([\hat{a}_{-k\downarrow}\hat{a}^+_{p+q\uparrow}\hat{a}_{p\downarrow}] + [\hat{a}_{-k\downarrow}\,\hat{a}^+_{p\downarrow}\hat{a}_{p+q\uparrow}])$$

$$= M\sum_p(\{\hat{a}_{-k\downarrow}\hat{a}^+_{p+q\uparrow}\}\,\hat{a}_{p\downarrow} - \hat{a}^+_{p+q\uparrow}\{\hat{a}_{-k\downarrow}\hat{a}_{p\downarrow}\} + \{\hat{a}_{-k\downarrow}\hat{a}^+_{p\downarrow}\}\hat{a}_{p+q} - \hat{a}^+_{p\downarrow}\{\hat{a}_{-k\downarrow}\hat{a}_{p+q\uparrow}\})$$

$$= M\hat{a}_{-k+q\downarrow}, \qquad (3.2.79)$$

$$[\hat{a}_{-k\downarrow,}\Delta_{sc}\sum_p(\hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow})] = \Delta_{sc}\sum_p([\hat{a}_{-k\downarrow}, \hat{a}^+_{p\uparrow}\hat{a}^+_{-p\downarrow}] + [\hat{a}_{-k\downarrow}, \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}])$$

$$= \Delta_{sc}(\{\hat{a}_{-k\downarrow}, \hat{a}^+_{p\uparrow}\}\hat{a}^+_{-p\downarrow} - \hat{a}^+_{p\uparrow}\{\hat{a}_{-k\downarrow}\hat{a}^+_{-p\downarrow}\} + 0)$$

$$= -\Delta_{sc}\hat{a}^+_{k\uparrow,} \qquad (3.2.80)$$

substituting eq. (3.2.78)– eq. (3.2.80) into eq. (3.2.77), we get

$$\omega \ll \hat{a}_{-k\downarrow,}\hat{a}_{k-q\downarrow} \gg = -\epsilon_{-k} \ll \hat{a}_{-k\downarrow,}\hat{a}_{k-q\downarrow} \gg + M \ll \hat{a}_{-k+q\downarrow}\hat{a}_{k-q\downarrow} \gg - \Delta_{sc} \ll \hat{a}^+_{k\uparrow}\,\hat{a}_{k-q\downarrow} \gg$$

$$(\omega - \epsilon_{-k}) \ll \hat{a}_{-k\downarrow,}\hat{a}_{k-q\downarrow} \gg = M \ll \hat{a}_{-k+q\downarrow}\hat{a}_{k-q\downarrow} \gg - \Delta_{sc} \ll \hat{a}^+_{k\uparrow}\,\hat{a}_{k-q\downarrow} \gg. \qquad (3.2.81)$$

From eq. (3.2.71), we obtain

$$\ll \hat{a}^+_{k-q\downarrow,}\hat{a}_{k-q\downarrow} \gg = \frac{1}{\omega+\epsilon_{k-q}} - \frac{M \ll \hat{a}^+_{k\uparrow}\hat{a}_{k-q\downarrow} \gg}{\omega+\epsilon_{k-q}} + \frac{\Delta_{sc} \ll \hat{a}_{-k+q\uparrow}, \hat{a}_{k-q\downarrow} \gg}{\omega+\epsilon_{k-q}}. \qquad (3.2.71.1)$$

From eq. (3.2.81), we obtain

$$\ll \hat{a}_{-k\downarrow}\hat{a}_{k-q\downarrow} \gg = \frac{M \ll \hat{a}_{-k+q\downarrow}\hat{a}_{k-q\downarrow} \gg}{\omega - \epsilon_{-k}} - \frac{\Delta_{sc} \ll \hat{a}^+_{k\uparrow}\hat{a}_{k-q\downarrow} \gg}{\omega - \epsilon_{-k}}. \qquad (3.2.81.1)$$

Substituting eq. (3.2.71.1) and eq. (3.2.81.1) into eq. (3.2.66), we get

$$\left((\omega + \epsilon_k) - \frac{M^2}{\omega+\epsilon_{k-q}} - \frac{\Delta^2_{sc}}{\omega - \epsilon_{-k}}\right) \ll \hat{a}^+_{k\uparrow}\hat{a}_{k-q\downarrow} \gg = -\frac{M}{\omega + \epsilon_{-k}} -$$

$$\left(\frac{M\Delta_{sc}}{\omega+\epsilon_{k-q}} + \frac{M\Delta_{sc}}{\omega - \epsilon_{-k}}\right) \ll \hat{a}_{-k+q\uparrow}, \hat{a}_{k-q\downarrow} \gg. \qquad (3.2.82)$$

Substituting eq. (3.2.71.1) and eq. (3.2.81.1) into eq. (3.2.76), we get

$$\left((\omega - \epsilon_{-k+q}) - \frac{M^2}{\omega-\epsilon_{-k}} - \frac{\Delta^2_{sc}}{\omega + \epsilon_{k-q}}\right) \ll \hat{a}_{-k+q\downarrow}\hat{a}_{k-q\downarrow} \gg = \frac{\Delta_{sc}}{\omega - \epsilon_{-k}} -$$

$$\left(\frac{M\Delta_{sc}}{\omega - \epsilon_{-k}} + \frac{M\Delta_{sc}}{\omega+\epsilon_{k-q}}\right) \ll \hat{a}^+_{k\uparrow}, \hat{a}_{k-q\downarrow} \gg. \qquad (3.2.83)$$

Appling nesting condition, $\epsilon_k = -\epsilon_{k\pm q} and\ \ \epsilon_{-k} = \epsilon_{-k\mp q}$, and using approximation $\epsilon_k = \epsilon_{-k}$, eq. (3.2.82) and eq. (3.2.83) respectively become

$$\left((\omega+\epsilon_k)-\frac{M^2}{\omega-\epsilon_k}-\frac{\Delta_{sc}^2}{\omega-\epsilon_k}\right) \ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = -\frac{M}{\omega-\epsilon_k} -$$

$$\left(\frac{M\Delta_{sc}}{\omega-\epsilon_k}+\frac{M\Delta_{sc}}{\omega-\epsilon_k}\right) \ll \hat{a}_{-k+q\uparrow}, \hat{a}_{k-q\downarrow} \gg . \qquad (3.2.84)$$

and

$$\left((\omega+\epsilon_k)-\frac{M^2}{\omega-\epsilon_k}-\frac{\Delta_{sc}^2}{\omega-\epsilon_k}\right) \ll \hat{a}_{-k+q\uparrow}, \hat{a}_{k-q\downarrow} \gg = \frac{\Delta_{sc}}{\omega-\epsilon_k} -$$

$$\left(\frac{M\Delta_{sc}}{\omega-\epsilon_k}+\frac{M\Delta_{sc}}{\omega-\epsilon_k}\right) \ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg . \qquad (3.2.85)$$

Let x= $\omega+\epsilon_k$ and y= $\omega-\epsilon_k$.

Then eq. (3.2.84) and eq. (3.2.85) respectively become

$$[\text{xy-}M^2\text{-}\Delta_{sc}^2] \ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = -M - 2M\Delta_{sc} \ll \hat{a}_{-k+q\uparrow}, \hat{a}_{k-q\downarrow} \gg \qquad (3.2.86)$$

and

$$[\text{xy-}M^2\text{-}\Delta_{sc}^2] \ll \hat{a}_{-k+q\uparrow}, \hat{a}_{k-q\downarrow} \gg = \Delta_{sc} - 2M\Delta_{sc} \ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg \qquad (3.2.87)$$

Derive for $\ll \hat{a}_{-k+q\uparrow}, \hat{a}_{-k\downarrow}^{+} \gg$ from $eq.$ (3.1.86) and substituting in eq. (3.1.87), then $\ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg$ is

$$\ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = \frac{-M[\text{xy}-M^2-\Delta_{sc}^2+2\Delta_{sc}^2]}{[(\text{xy}-M^2-\Delta_{sc}^2)^2]-[2M\Delta_{sc}]^2}$$

$$\ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = \frac{-M[\omega^2-\epsilon_k{}^2-M^2+\Delta_{sc}^2]}{[(\omega^2-\epsilon_k{}^2-M^2-\Delta_{sc}^2)^2]-[2M\Delta_{sc}]^2}$$

$$\ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = \frac{-M[\omega^2-\epsilon_k{}^2-M^2+\Delta_{sc}^2]}{[\omega^2-\epsilon_k^2-(\Delta_{sc}+M)^2][\omega^2-\epsilon_k^2-(\Delta_{sc}-M)^2]} . \qquad (3.2.88)$$

Using the expression $\omega \to i\omega_n$,we obtain

$$\ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = \frac{-M[\omega^2-\epsilon_k{}^2-M^2+\Delta_{sc}^2]}{[\omega_n^2+\epsilon_k^2+(\Delta_{sc}+M)^2][\omega_n^2+\epsilon_k^2+(\Delta_{sc}-M)^2]} \qquad (3.2.89)$$

after some rearrangement eq. (3.2.88) can be expressed as

$$\ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = \frac{-1/2(\Delta_{sc}+M)}{\omega_n^2+\epsilon_k^2+(\Delta_{sc}+M)^2} + \frac{1/2(\Delta_{sc}-M)}{\omega_n^2+\epsilon_k^2+(\Delta_{sc}-M)^2} , \qquad (3.2.90)$$

we express $\Delta_j(k) = \Delta_{sc} - (-1)^j M$, where, $\Delta_j(k)$ is effective order parameter,

$$\ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = \frac{-1/2\Delta_j(k)}{\omega_n^2 + \epsilon_k^2 + \Delta_j^2(k)} + \frac{1/2\Delta_j(k)}{\omega_n^2 + \epsilon_k^2 + \Delta_j^2(k)} \quad (3.2.91)$$

$$\ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = \frac{1}{2}\sum_{j=1,2} \frac{(-1)^j\Delta_j(k)}{\omega_n^2 + \epsilon_k^2 + \Delta_j^2(k)}\,. \quad (3.2.92)$$

From Matsubara's frequency, we have

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

Inserting the above expression into eq.(3.2.92), we get

$$\ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg = \frac{1}{2}\sum_{j=1,2} \frac{(-1)^j\beta^2\Delta_j(k)}{(2n+1)^2\pi^2 + \beta^2(\epsilon_k^2 + \Delta_j^2(k))}\,. \quad (3.2.93)$$

The SDW order parameter M is given by

$$M = \frac{U}{\beta}\sum_{\mathrm{k,n}} \ll \hat{a}_{k\uparrow}^{+}\hat{a}_{k-q\downarrow} \gg. \quad (3.2.94)$$

Insert eq. (3.2.93) into eq. (3.2.94), we get

$$M = -\frac{U}{2}\sum_{k,n,j=1} \frac{\beta\Delta_j(k)}{(2n+1)^2\pi^2 + \beta^2(\epsilon_k^2 + \Delta_j^2(k))}\;, \qquad \text{where } \mathrm{j} = 1 \quad (3.2.95)$$

use the equality below, where $\gamma = \beta(\epsilon_k^2 + \Delta_1(k)^2)^{\frac{1}{2}}$

$$\sum_{-\infty}^{\infty} \frac{1}{(2n+1)^2\pi^2 + \gamma^2} = \frac{\tanh\gamma/2}{2\gamma} \quad (3.2.96)$$

substituting eq. (3.2.96) into eq. (3.2.95), we obtain

$$M = \frac{-U}{4}\sum_{j=1} \frac{\Delta_j(k)\tanh\frac{\beta}{2}(\epsilon_k^2 + \Delta_j^2(k))^{\frac{1}{2}}}{(\epsilon_k^2 + \Delta_j^2(k))^{\frac{1}{2}}}. \quad (3.2.97)$$

Converting the summation over k values into an integral with the cut-off energy from $\pm\hbar\omega_b$ measured from the Fermi level and use the density of state at the Fermi level is N(o). We assume the density of state is $N(0) = 2N(0)_j$. So for j=1

$$M = \frac{-N(O)U}{4}\int_{-\hbar\omega_b}^{\hbar\omega_b} \frac{\Delta_j(k)\tanh\frac{\beta}{2}(\epsilon_k^2+\Delta_j^2(k))^{\frac{1}{2}}}{(\epsilon_k^2+\Delta_j^2(k))^{\frac{1}{2}}}\, d\epsilon_k \qquad (3.2.98)$$

$$M = \frac{-N(0)_j U}{2}\int_{-\hbar\omega_b}^{\hbar\omega_b} \frac{\Delta_j(k)\tanh\frac{\beta}{2}(\epsilon_k^2+\Delta_j^2(k))^{\frac{1}{2}}}{(\epsilon_k^2+\Delta_j^2(k)^{\frac{1}{2}}}\, d\epsilon_k$$

Let $\lambda_j = N(0)_j U$

$$M = -\lambda_j\Delta_j \int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}(\epsilon_k^2+\Delta_j^2(k))^{\frac{1}{2}}}{(\epsilon_k^2+\Delta_j^2(k))^{\frac{1}{2}}}\, d\epsilon_k \qquad (3.2.99)$$

We can solve above equation by the same technique used in order to solve the first term of the right hand side of eq. (3.2.49) and, we obtain

$$M = -\lambda_j\Delta_j\left(\left(\ln 1.14\frac{\hbar\omega_b}{k_\beta T_{sdw}}\right) - {\Delta_j}^2\left(\frac{1}{\pi k_\beta T_{sdw}}\right)^2 1.052\right) \qquad (3.2.100)$$

For very small value of Δ_j the second term of the RHS of eq (3.1.100) goes to zero

$$M = -\lambda_j\Delta_j\left(\ln 1.14\frac{\hbar\omega_b}{k_\beta T_{sdw}}\right) \qquad (3.2.101)$$

Rearranging eq. (3.2.101) , we obtain

$$T_{sdw} = 1.14\frac{\hbar\omega_b}{k_\beta}\exp\left(\frac{M}{\lambda_j\Delta_j}\right) \qquad (3.2.102)$$

Chapter 4

Result and Discussion

In this chapter, we described the effect of temperature (T) on superconducting order parameter (Δ_{sc}). We also examined the effect of magnetic order parameter (M) on superconducting transition temperature (T_c) and on SDW transition temperature (T_{sdw}) in $SmO_{1-x}F_xFeAs$. In chapters two and three, using the model of the Hamiltonian and retarded double time temperature dependent green's function formalism, we obtained mathematical expression for superconducting transition(critical) temperature (T_c), the superconducting order parameter (Δ_{sc}), the magnetic order parameter(M), and spin density wave transition temperature (T_{sdw}). From eq. (3.2.48) we have got the superconducting transition (critical) temperature for the superconductor $SmO_{1-x}F_xFeAs$. Using this T_c value and eq. (3.2.61), we plot the phase diagram of Δ_{sc}versus T which is shown in figure 4.1. As seen in this figure, when the temperature increases the superconducting order parameter decreases and vanishes as the temperature is equal to the critical temperature. Based on eq. (3.2.46.1) we plotted the phase diagram of T_c versus M (fig 4.2). This figure indicates, as the magnetic order parameter (M) increases the superconducting transition temperature (T_c) decreases. The phase diagram of magnetic ordering temperature (T_{sdw}) versus magnetic ordering (M) also plotted (fig 4.3) based on the eq. (3.2.102). As we observed from this graph the magnetic transition temperature is increases (directly proportional) as the magnetic order parameter increases. And finally, we merged fig (4.2) and fig (4.3), to indicate the region where both orders i.e. superconductivity and spin density wave are coexisted (Fig. 4.4).

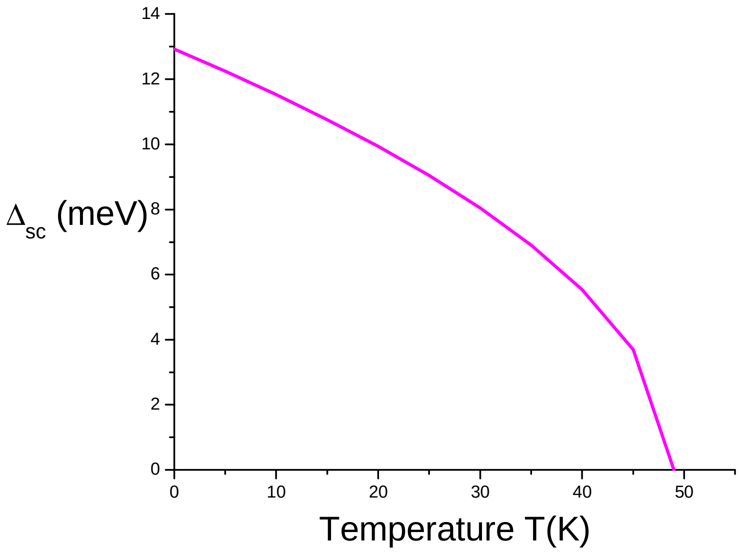


Figure 4.1: Superconducting order parameter vs. temperature for pure $SmO_{1-x}F_xFeAs$ superconductor.

As seen in this figure, when the temperature increases the superconducting order parmameter decreases and vanishes as the temperature is equal to the critical temperature.

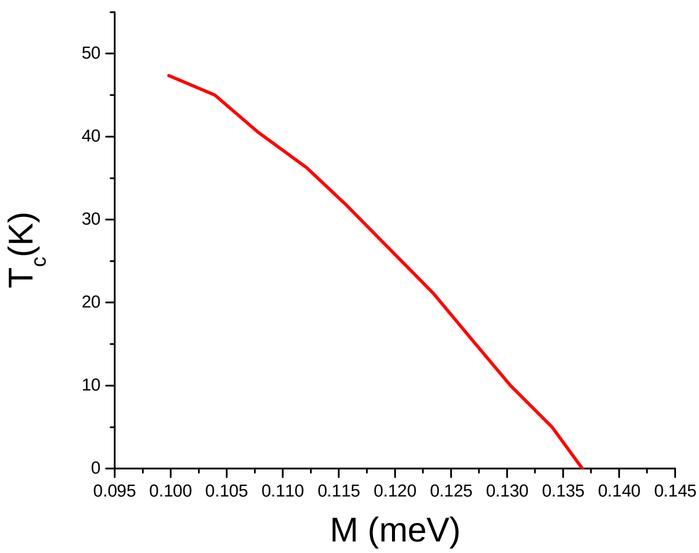


Figure 4.2: superconducting critical temperature vs. magnetic order parameter.

The above figure indicates, as the magnetic order parameter (M) increases the superconducting transition temperature (T_c) decreases.

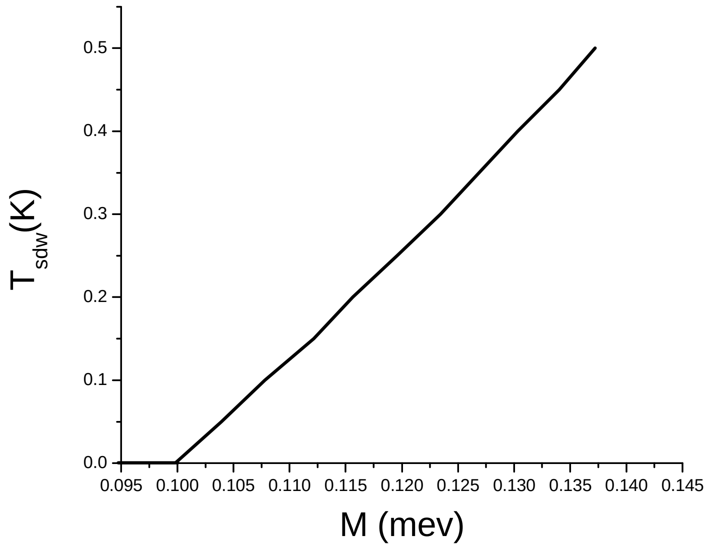


Figure 4.3: spin density wave transition temperature (T_{sdw}) vs. magnetic order parameter.

This figure shows that the magnetic transition temperature increases as the magnetic order parameter increases.

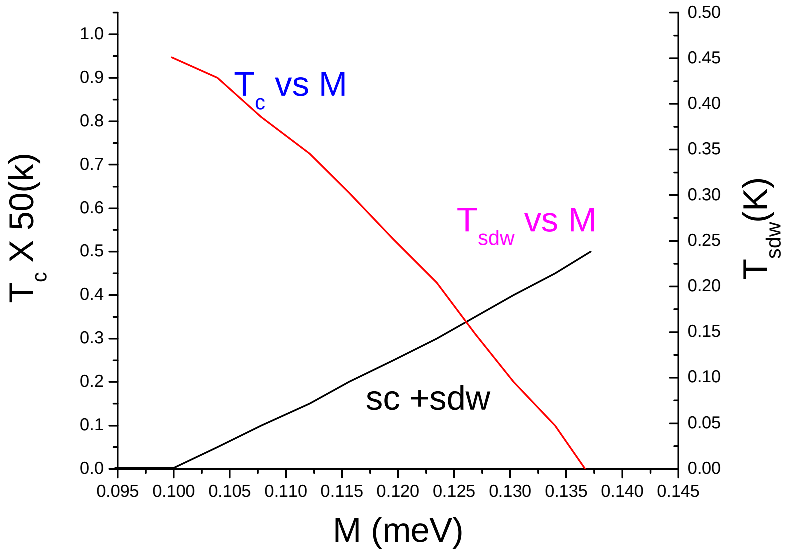


Figure 4.4: the superconducting critical temperature and SDW transition temperature vs. magnetic order parameter.

The above figure shows that the coexistence of superconductivity and spin density wave.

Chapter 5

Conclusion

In this work, we have studied the possible coexistence of superconductivity and spin density wave in $SmO_{1-x}F_xFeAs$. Using Hamiltonian model and Green's function formalism we obtained mathematical expression for superconducting order parameter(Δ_{sc}), magnetic order parameter (M), critical temperature (T_c), and SDW transitional temperature (T_{sdw}). Based on these mathematical expressions we plotted the three graphs (Δ_{sc} vs. T, Tc vs. M, T_{sdw} vs. M) and finally the last two graphs (Tc vs. M and T_{sdw} vs. M) were merged to obtain the coexistence of superconductivity and SDW. The result of our work described: a) as temperature increases superconducting order parameter decreases. b) when magnetic order parameter increases the critical temperature decreases c) while the magnetic order parameter increases with the SDW transitional temperature. Moreover, the region under the intersection of the two merged graphs (fig 4.4) shows that superconductivity and spin density wave coexist in $SmO_{1-x}F_xFeAs$.

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Declaration

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

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