

# COEXISTENCE OF SPIN DENSITY WAVE AND SUPERCONDUCTIVITY

A thesis submitted to the School of Graduate Studies  
Addis Ababa University



In partial Fulfilment of the Requirements for the  
Degree of Master of Science in Physics

By

**Kumneger Tadele**

Addis Ababa, Ethiopia

July 2007

**ADDIS ABABA UNIVERSITY**  
**FACULTY OF SCIENCE**  
**DEPARTMENT OF PHYSICS**

The undersigned hereby certify that they have read and recommended to the Faculty of Science School of Graduate Studies for acceptance a thesis entitled “**Coexistence of Spin Density Wave And Superconductivity**” by **Kumneger Tadele** in partial fulfillment of the requirements for the degree of **Master of Science in Physics**.

Name	Signature
Prof. P. Singh, Advisor	-----
Dr. H. S. Tewari, Examiner	-----
Dr. Tesgera Bedassa, Examiner	-----

*This work is dedicated to the memory of my beloved parents  
Tadele Gemechu and  
Aregash Demessa  
for their constant encouragement and support over all my life.*

## Acknowledgements

First of all and foremost I would like to thank the Almighty God for His Grace and blessing on me during all of my life.

I would like to express my sincere gratitude to my advisor Prof. P. Singh for his unlimited and constructive guidance, advice, suggestions and comments. I am also thankful Dr. Ramanand Jha for his many suggestions and support.

I am grateful to all my families especially to my parents Tadele Gemechu and Aregash Demessa for their patience and *love*. Without them this work would never have come into existence.

I am thankful to my all friends Abera Debebe, Samuel Takele, Birhanu Asmerom, Abrar Demsses, Zerihun, Ygeremu, Behilu, Hileyesus and all those whose names could not be mentioned for their help and cooperation and for all the good and bad times we had together.

Finally, I would like to thank the Ministry of education for the sponsorship they granted me to join the school of Graduate studies.

Addis Ababa, Ethiopia

Kumneger Tadele

July 2007

# Table of Contents

Table of Contents	vi
List of Figures	viii
Introduction	1
<b>1 The General Overview of Superconductors</b>	<b>5</b>
1.1 Introduction . . . . .	5
1.2 BCS ground state . . . . .	8
1.3 Meissner-Ochsenfeld Effect . . . . .	9
1.4 Conventional and Unconventional Superconductors . . . . .	12
1.5 Spin Density Wave and Charge Density wave . . . . .	14
1.6 Coexistence state . . . . .	18
<b>2 Mathematical Techniques</b>	<b>24</b>
2.1 Introduction . . . . .	24
2.2 Effective Electron-Electron Interaction . . . . .	24
2.3 Green's Function . . . . .	30
2.3.1 Double-Time Temperature-Dependent Green's Function . . . . .	33
<b>3 Mathematical Formulation Of The Problem</b>	<b>37</b>
3.1 Coexistence Of SDW and Singlet Superconductivity . . . . .	37
3.1.1 The order parameter of SDW . . . . .	38
3.1.2 The order parameter of superconductivity . . . . .	43
3.2 Coexistence of SDW and Triplet Superconductivity . . . . .	45
3.2.1 Superconducting Order Parameter . . . . .	46
3.2.2 SDW Order Parameter . . . . .	49
<b>4 Results And Discussion</b>	<b>51</b>

<b>5 Conclusion</b>	<b>55</b>
<b>Bibliography</b>	<b>56</b>
<b>Declaration</b>	<b>59</b>

# List of Figures

1.1	Meissner-ochsenfeld effect in superconductors. (a)If a normal metal is first cooled and then placed in a magnetic field, it will expel the field. (b) If a normal sample in a magnetic field is cooled, then the field will be expelled from the system. . . . .	11
1.2	Peierls distortion in a one-dimensional metal with a half-filled band .	19
1.3	Pressure temperature phase diagram of $(TMTSF)_2PF_6$ in the 8-11kbar range . . . . .	21
4.1	Thermal variation of SS gap and SDW gap . . . . .	54
4.2	The variation of TSC gap and SDW gap with temperature . . . . .	54

## Abstract

Superconductivity and magnetism usually try to avoid each other. This feature can be exploited to, for example, levitate a magnet above superconductor. The discovery of magnetic materials that are also superconductors has reconciled these two physical phenomena that were previously thought to be incompatible. The recent discovery of compounds that are both ferromagnetic and superconducting at the same time came as a surprise to many physicists. The mechanism of superconductivity in these superconductors is not known. There are suggestions of spin fluctuations as mediating superconductivity. In the present work we examine the possible coexistence of spin density wave and superconductivity. For this we have obtained expressions which relate the order parameters of these two states. Both singlet and triplet superconductivity are considered. The diagrams show the variation of the order parameters  $\Delta_{SC}$  and  $\Delta_{SDW}$  with temperature and also the coexistence region of SDW and superconductivity.

# Introduction

Superconductivity, a phenomenon which occurs in certain materials and is characterized by the absence of electrical resistivity, was discovered in 1911 in Leiden by Kamerlingh Onnes when he noticed that the resistivity of Hg metal vanished abruptly at about 4.2k. A critical temperature at which resistance vanishes will reduce with magnetic field, that means superconductivity will be destroyed by strong magnetic field and the maximum field that can be applied to a superconductor at a particular temperature and still maintain superconductivity is called critical field. Another fundamental property of the superconducting state was discovered in 1933 when Meissner and Ochsenfeld demonstrated that magnetic flux is expelled from the interior of a sample of superconductor which ensures that superconductivity is a manifestation of quantum mechanics. A great deal was known about superconductivity in 1950's and it is proved that the responsible phenomenon for superconductivity is electron-phonon interaction. Leon Cooper laid down the base for this clue when he showed that the non-interacting Fermi sea is unstable towards the addition of a single pair of electrons with attractive interactions and the microscopic mechanism of superconductivity was discovered in 1957 by Bardeen, Cooper and Schrieffer. Cooper pairs, which take the responsibility for superconducting phenomena, are capable of

passing from one superconductor to another without resistance when two superconductors are joined by a thin, insulating layer, and it is called dc Josephson effect. Until 1986 the critical temperatures were always less than 23k. But in 1986 Bednorz and Muller discovered high  $T_c$  superconductivity in ceramic materials, and this work is recognized with 1987 Nobel prize.

Generally superconductivity and magnetism are exclusive phenomena. For a long time it was believed that they are enemies to each other, while later on different workers have made predictions over the possible coexistence of these two states. Ferromagnetism (FM) and superconductivity (SC) are basically characterized by mutual repulsion. After Ginzburg realizes possible coexistence of the two states under the condition that the magnetization is less than the thermodynamic critical field, many experimental investigations have been performed. The first successful experiment was performed by Matthias et al. who studies impurity ferromagnetism in a superconductor [1].

With the discovery of triplet superconductivity in  $UGe_2$ ,  $URhGe$  and  $ZrZn_2$  [2] the speculation is ripe towards spin fluctuation mediated superconductivity in the systems in view of magnetically induced superfluidity in  $^3He$  [3]. And then competition or coexistence of magnetic order and superconductivity arise as a very important problem in condensed matter physics and it has intrigued both experimentalists and theoretician for a long time. Different systems have magnetic order and superconductivity in close vicinity. For example copper oxide superconductors display singlet superconductivity next to antiferromagnetism(AF) [4]. For the existence of triplet superconductivity in Strontium Ruthenate,  $Sr_2RuO_4$ , proximity to ferromagnetism

is necessary [ref.5]. Moreover the recent discovery of superconductivity near ferromagnetism in  $ZrZn_2$  and  $UGe_2$  have stimulated a debate on the coexistence of ferromagnetism and triplet superconductivity(TS) [2]. It was surprising to find superconductivity in  $UGe_2$  coexisting with ferromagnetism and its destruction above the critical pressure with loss of ferromagnetism. FM and superconductivity comes from the same localized U 5f electrons. At ambient pressure  $UGe_2$  has a character of ferromagnetism whose transition temperature,  $T_{FM}$ , decrease gradually with increasing pressure and when the value of pressure exceeds 1Gpa SC starts to appear with increasing  $T_c$ . The odd-parity superconductivity can occur in the ferromagnetic state of  $UGe_2$  quite generally when ferromagnetic fluctuations are large enough and when crystals can be made sufficiently pure to avoid the pair breaking influence of defects.

Different experiments on quasi one-dimensional superconductors in high magnetic fields have proved that triplet superconductivity is highly affected by the antiferromagnetic phase or insulating SDW order [5]. These experiments together with the P-T phase diagram of quasi one-dimensional  $(TMTSF)_2PF_6$  can lead to a new non-uniform phase for quasi one-dimensional systems where AF and TS coexist. Ferromagnetic component of the magnetic order is present at a pressure and temperature where superconductivity is found [2]. The pressure above which superconductivity in  $UGe_2$  disappears,  $P_c \simeq 16kbar$ , coincides with the pressure where ferromagnetism is also suppressed or destroyed. This leads us to the conclusion that superconductivity and ferromagnetic order are cooperative phenomena in this compound [2]. In itinerant systems the same electrons (for example d-electrons in a transition metal) are responsible for both superconductivity and ferromagnetism which suggest possible coexistence state in such systems [6].

Generally superconductivity characterized by the existence of permanent macroscopic currents which has a tendency to oppose magnetic fields. Thus superconductivity, to compete with ferromagnetism, must be spatially modulated such that act as a virtual mixed state of a conventional superconductor and applied field even in the absence of applied external field.

In present work we have tried to investigate the possibilities for coexistence of superconducting state and SDW ordering. In the first chapter the general behavior of superconducting state and CDW/SDW order are briefly discussed. And both experimental results and theoretical views about the coexistence state are discussed there. The second chapter is going to explain the mathematical techniques that we have used in the next chapter to obtain an expression in which the order parameters of both states are involved and to discuss the interaction term in the Hubbard model. In the third chapter we formulate the problem and present the calculational details. Chapter four is devoted to discuss and conclude the final results.

# Chapter 1

## The General Overview of Superconductors

### 1.1 Introduction

The Helium gas was discovered on earth at the turn of the 20<sup>th</sup> century, which is about four decades later to its discovery in the chromosphere of the sun when unusual spectral lines were observed from the emitted light of the hot incandescent gases [7]. And later on in 1908 Kamerling Onnes succeeded in liquifying this gas at a temperature a few degrees above absolute zero, which facilitate the study of metallic conductivity at very low temperature.

In 1911 Onnes observed that the electrical resistance of Mercury drops almost discontinuously to zero at a temperature of about 4.2k, and, he had concluded that "Mercury has passed in to a new state which, on account of its remarkable electrical properties, he called the superconductive state" [8]. The temperature at which the transition takes place is called critical temperature,  $T_c$ . Then the problem of discovering new superconducting materials with higher  $T_c$  was immediatly offer the discovery. The critical temperature of  $Nb_3Ge$  was found to be 23k in 1973 which remains the highest critical temperature until 1986 when high  $T_c$  superconductivity was discovered

by Bednorz and Muller in  $La_{2-x}Ba_xCuO_4$  at 35k. At present the highest  $T_c$  is about 160k in Hg based superconductor. The critical temperature,  $T_c$ , of superconductor varies with isotopic mass as;

$$M^\alpha T_c = constant$$

which is indicative of the involvement of lattice vibrations or phonons in the phenomenon of superconductivity [9].

Superconductivity is a bulk property of solids. According to London the superconducting phenomenon was ascribed to a condensation of the electrons in momentum space. Bulk superconductors show Meissner effect, i.e ; magnetic induction  $\mathbf{B}$  is always zero inside it, and it falls from its external value to zero in a distance  $\lambda$  called penetration depth, given by

$$\lambda = c \sqrt{\frac{m}{4\pi n_s e^2}}$$

Where;

$\mathbf{m}$  =mass of an electron

$n_s$  =density of superconducting electrons

$\mathbf{e}$  =charge of an electron

$\mathbf{c}$  =speed of light

There fore the only field that is allowed in pure superconducting state is exponentially damped as we go in from an external surface and it, mathematically, can be expressed as;

$$\mathbf{B}(x) = \mathbf{B}(0) \exp\left(\frac{-x}{\lambda}\right)$$

The second length involved in a superconducting system is called coherence length,  $\xi$ , which is the distance over which the electrons have coherence or the range of the wave function that described the superconducting state.

superconductivity can be destroyed not only by increasing the temperature but also by applying a sufficiently strong magnetic field. This is because the macroscopic magnetization depends upon aligning the electron spins parallel to one another, while superconductivity depends upon pairs of electrons with their spins antiparallel. Hence, since the Cooper pairs of electrons in the BCS theory have a very small binding energy, the external magnetic fields exert torques on the electron spins which tend to break up these pairs. The critical field in which superconductivity is destroyed decreases with increasing temperature and its dependence on temperature given by the formula

$$\mathbf{H}_c(T) = \mathbf{H}_c(0)[1 - (\frac{T}{T_c})^2] \quad (1.1.1)$$

superconductor can also be destroyed by the induced supercurrent if it exceeds a "critical current", which can produce a magnetic field that is greater than critical field,  $H_c$ , and the phenomenon is called 'Silsbees' effect [9].

In an ideal superconductor, electrons form cooper pairs which flow in coherent manner without resistance. The situation is much different in the case of "dirty" superconductors. One type of "dirty" superconductors are thin film materials that are strongly disordered - without the nice periodic atomic arrangements of crystalline materials. In "dirty" superconductors, cooper pairs can be so strongly scattered by random disorder that they loose their coherence and become immobile. In this limit a "dirty" superconductor becomes an insulator - its resistance can increase sharply with decreasing temperature. If one can turn a "knob" to restore the coherence

destroyed by disorder, then it is possible to tune a dirty superconductor between a high resistance insulating state and a zero resistance superconducting state resulting in a superconducting switching device. A dc electric current and electric field are possible knobs, where the later one is used to control field effect transistors in a computer [10].

## 1.2 BCS ground state

Cooper tried to understand the response of a system of filled Fermi sea when two more electrons are added to it [8, 11]. He supposed that the electrons within the Fermi sea held rigidly in their states so that these states are forbidden by the exclusion principle to the two extra electrons. However the electrons within the Fermi sea have the probability to be scattered above. One of the possibilities that the two electrons lie just at the fermi level is that the superposition of their states above the Fermi sea. If the energy in this state have negative value the pair of electrons will tend to form a bound state. In this case the fermi sea will be unstable and the electrons will tend to form a new state which is lower in energy than that obtained by adding them to the top of the Fermi sea. Thus one can form a state with lower energy by removing a pair of electrons from the completely filled Fermi sea and allowing them to occupy a superposition of states above it. But removing many pairs will result in invalidity of discussing the pairs independently, since they can interfere with each other.

BCS state is a quantum mechanical state of a system of attractively interacting electrons inside the metal. Electrons move independently in the normal metal while in BCS state they are bound in to cooper pairs by the attractive interactions. Hence, the

theory of superconductivity involves a net attractive interaction between electrons in the neighborhood of the fermi surface. Although the direct electrostatic interaction is repulsive, it is possible for the ionic motion to "over screen" the coulomb interaction, leading to a net attraction. Allowing the ions to move in response to motions of the electrons led to a net interaction between electrons with wave vectors  $\mathbf{k}$  and  $\mathbf{k}'$ .

It is mainly the interaction between electrons and phonons which is responsible for the superconducting transition. This interaction leads indirectly to a retarded interaction between electrons, and, for electrons near the Fermi surface, this interaction is attractive and will tend to lower the energy of the system. If the attraction is sufficiently strong, in comparison with the coulomb repulsive interaction, the electrons tend to go in to a new state which posses the properties of a superconductor and is called superconducting state. The retarded interaction between the electrons [8, 9, 12] can be approximated to:

$$V_{ph} = \frac{1}{2} \sum_{k,k',q,\sigma,\sigma'} \left( \frac{\hbar\omega_q |g|^2}{(\varepsilon_k - \varepsilon_{k+q})^2 - (\hbar\omega_q)^2} C_{k+q,\sigma}^+ C_{k'\sigma'}^+ C_{k'+q,\sigma'} C_{k,\sigma} \right) \quad (1.2.1)$$

and the interaction will be attractive as long as

$$|\varepsilon_k - \varepsilon_{k+q}| < \hbar\omega_q$$

Hence only the electrons near the fermi surface with in the energy range  $\pm\hbar\omega_q$  are responsible for superconductivity.

### 1.3 Meissner-Ochsenfeld Effect

Superconductivity will not be defined completely by the concept of zero resistivity, but by Meissner-Ochsenfeld effect, which demonstrate the fact that a superconductor

expels a weak external magnetic field. Consider a sample of a material in its normal state,  $T > T_c$ , and placed in zero external field. If we first cool the sample to a temperature below  $T_c$  keeping the field zero, the material will make a phase change from normal to superconductor. Then if we gradually turn on the external field, the field inside the sample must remain zero as long as the external field is weak, less than the critical field that can penetrate a superconductor.

On the other way if we consider the sample in a temperature above  $T_c$  and we first turn on the external field, the field will easily penetrate in to the sample. If we now cool the sample below  $T_c$ , the sample will change a phase from normal to superconductor. To account for Meissner-Ochsenfeld effect, the superconductor will actually manage to remove the now present magnetic field from its interior by spontaneously running electric currents on the surface where no currents existed a moment before. The direction of the currents is such as to create an opposing magnetic field to cancel the one present, which is not the case for perfect diamagnet in which the already existing steady magnetic field would be expected to remain, this is because of the fact that conductors do not like any form of change in magnetic fields. Hence the active exclusion of magnetic field is an effect distinct from zero resistance and the phenomenon is illustrated in fig. 1.3 [13]. Hence Meissner effect not only implies the magnetic fields are excluded from superconductors but also that any field originally present in the metal expelled from it when lowering the temperature below its critical value.

However, in type-II superconductors Meissner effect is incomplete. The magnetic field is not excluded completely but constrained in filaments within the material and they are in the normal states surrounded by supercurrents. In the material of such

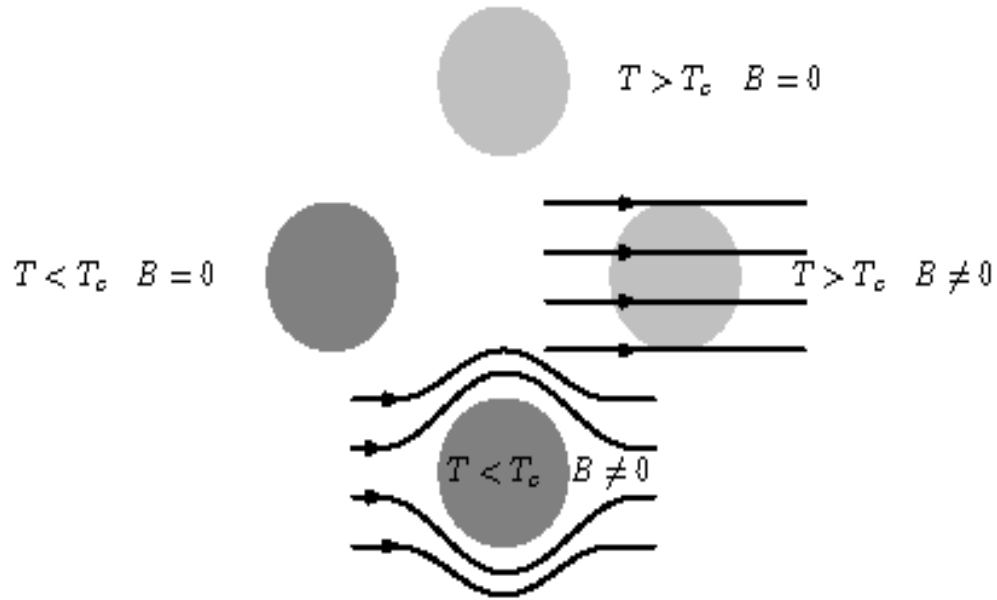


Figure 1.1: Meissner-ochsenfeld effect in superconductors. (a) If a normal metal is first cooled and then placed in a magnetic field, it will expel the field. (b) If a normal sample in a magnetic field is cooled, then the field will be expelled from the system.

kind, transition from superconducting to normal state due to applied field will extend over an interval of magnetic fields rather than undergoing a phase transition suddenly at a point called critical field like that of type-I, and in this interval the magnetic field will partially penetrate the superconductor and the material is called in mixed state or vortex state which adjoins the superconducting phase below the lower critical field  $H_{c1}$  and the normal phase above the upper critical field  $H_{c2}$ . Such materials remain superconducting under high magnetic field. For type-II superconductors, the magnetic field penetrates in to the specimen in the form of vortex lines, each carrying a quantized flux, in the mixed state. Scanning the magnetic field back and forth result

with hysteresis in the presence of flux pinning by defects or impurities. The hysteresis is indicative of the flux pinning or equivalently the maximum current density that the superconductor can carry before driving it to the normal state. To the account of M. D. Lan and colleagues measurement the hysteresis loop tilted with magnetic ions, which leads them to the concept of the possible coexistence of the paramagnetism and superconductivity [14].

Meissner effect suggests that superconductors act as a perfect diamagnet; magnetic fields are actively excluded from superconductors. If a small magnet is brought near a superconductor, it will be repelled by mirror images of each pole that are produced by induced supercurrents. This means a small permanent magnet can be levitated by this repulsive force if it is placed above a superconductor and the phenomenon is called Magnetic levitation. It is possible to cause to oscillate or rotate the suspended magnet by tapping it with a sharp instrument but the motion is damping and will come to rest in a few seconds though the magnet is continuously suspended and the motion could be modeled as a damped sine wave;

$$\theta(t) = \exp(-\alpha t) \sin(\omega t) \quad (1.3.1)$$

The damping is from eddy currents which are believed to be in the magnet itself.

## 1.4 Conventional and Unconventional Superconductors

Conventional superconductivity is characterized by s-wave Cooper pairs, formed by a net isotropic attractive interaction originating from the electron-phonon interaction, which is consistent with BCS theory. For s-wave superconductor the phase

of  $\Delta(\mathbf{k})$  is constant irrespective of the direction of  $\mathbf{k}$ . In conventional superconductors spin-orbit interaction is negligible. The paired electrons should possess finite relative orbital angular momentum in order to reduce strong on-site coulomb repulsion which is a key ingredient in strong electronic correlation. And this remark the close relationship between strong correlations and unconventional superconductivity. The order parameter of conventional superconductors show the full lattice symmetry. While in the case of unconventional superconductor the symmetry will broken and the superconducting gap vanishes some where on the Fermi surface [15].

Unconventional superconductors are materials that display superconductivity but that do not conform to BCS theory and Nikolay Bogolyubov theory. A state with odd parity in a crystal with inversion symmetry does always lead to an unconventional superconducting state. The first unconventional triplet superconductor discovered by Denis Jerome and Klaus Bechgaard in 1979 is  $(TMTSF)_2PF_6$ . Recent experiments confirm unconventional triplet nature of superconducting pairing in  $(TMTSF)_2X$ . The first high  $T_c$  superconductor, Lanthanum based cuprate perovskite, that discovered by Bednorz and Muller in 1986, for which they have got nobel prize in 1987, is also unconventional singlet d-wave superconductor. The origin of the attractive force leading to the formation of pairs in high  $T_c$  superconductors is different from that of in BCS theory. The fact that the superconducting temperature region lies close to that in which the antiferromagnetic ordering is displayed for TMTSF salts has suggested that the electron pairing mechanism is mediated by a fluctuating SDW. An attractive interaction between electrons mediated by ferromagnetic(so-called paramagnons) or antiferromagnetic(so-called antiparramagnons) spin fluctuation is essentially anisotropic and leads to the formation of cooper pairs with a non-zero angular

momentum. The anisotropic pairing of the cooper pair is usually referred to as the unconventional superconductivity. The highest critical temperature so far achieved in a conventional superconductor is 39k in magnesium diboride. The most successful theory of conventional superconductivity up to date, called BCS theory of superconductivity, can be extended to describe the mechanism in unconventional superconductors simply by assuming the possibility of an anisotropic wave function of the cooper pair [11].

## 1.5 Spin Density Wave and Charge Density wave

Spin density wave is broken-symmetry ground state of metal which is thought to arise as the consequence of electron-electron interactions. This state has many similarities to the other broken-symmetry ground states of metals, such as superconductivity and charge density waves. In all cases the ground state is that of the coherent superposition of pairs. SDW refers to the periodic modulation of spin density with period,  $T = \frac{\pi}{k_F}$ , determined by Fermi wave number  $k_F$  [16]. The SDW state is a kind of antiferromagnetic state, with the electronic spin density forming a static wave. The density varies perpendicularly 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. Generally normal state is characterized by the density of electrons with spin up  $\rho_{\uparrow}(\mathbf{r})$  is completely cancelled by spin down electron density  $\rho_{\downarrow}(\mathbf{r})$ . While SDW state have finite resultant density  $\sigma(\mathbf{r}) = \rho_{\uparrow}(\mathbf{r}) - \rho_{\downarrow}(\mathbf{r})$  and it is a function of position vector  $\mathbf{r}$  of the SDW state [17]. The ground states of CDW and SDW are the coherent superposition of electron-hole pairs and they are not uniform rather

displays a periodic spatial variation.  $CDW_s$  were first discussed by Frohlich in 1954 and Peierls in 1955. SDW states were postulated by Overhauser in 1962. It was recognized early that highly anisotropic band structures are important in leading to these ground states. Experimental evidence for these ground states was found much later, when materials with a linear chain structure and metallic properties were discovered and investigated. Such SDW ground state can be formed when a system possesses nested pieces of Fermi surface together with intermediate Coulomb correlation. In quasi one-dimensional metals the SDW ground state can be represented by an expression;

$$\Delta S(a) = \Delta S_0 \cos(2k_F a + \phi)$$

where  $\Delta S(a)$  is spin modulation along the chain direction  $a$  [16]

$SDW_s$  are marked by a periodic spin density modulation. It can be either commensurate or incommensurate with the background crystal lattice. Its origin can be electron-hole pairing or finite wavevector singularities of the magnetic susceptibility.  $SDW_s$  with the inherent wavevector  $\mathbf{Q}$  were suggested by Overhauser for isotropic metals [18]. It is Fermi surface nesting that is responsible for SDW stabilization.

X-ray scattering experiments in Cr, which is and whose alloys are the most common hosts of SDW, reveal second and fourth harmonics of periodic lattice distortions accompanied by  $CDW_s$  observed simultaneously with the basic SDW magnetic peaks at the incommensurate wavevector  $\mathbf{Q}$ ; the incommensurability being determined by the size difference between electron and hole Fermi surfaces [19].

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. Hence one can present a model, to study the coexistence of superconductivity and SDW, that incorporates two competing physical processes involving electron-hole (SDW) like pairing of opposite spins with a net momentum difference ( $\mathbf{Q}$ ) between the conjugates and electron-electron (superconducting) pairing of opposite spins with total momentum zero. The simplest model one can use to describe the anti ferromagnetic ordering of the two dimensional correlated system is the Hubbard model on a square lattice [17]. And it is given by;

$$H = - \sum_{i,j,\sigma} t_{ij} C_{i\sigma}^+ C_{j\sigma} + U \sum_i C_{i\uparrow}^+ C_{i\uparrow} C_{i\downarrow}^+ C_{i\downarrow}$$

Where;

$t_{ij}$  = hopping integrals between the different orbitals i and j

$U$  = onsite coulomb repulsion

$C^+(C)$  = creation(anhilation) operator

With this the mean field Hamiltonian for a transverse SDW state can be;

$$H_{SDW} = \sum_{k\sigma} (\varepsilon_k - \mu) C_{k\sigma}^+ C_{k\sigma} + \Delta_{SDW} \sum_k C_{k+Q\uparrow}^+ C_{k\downarrow} + C_{k\downarrow}^+ C_{k+Q\uparrow} \quad (1.5.1)$$

Where the order parameter of SDW,  $\Delta_{SDW}$ , is given by;

$$\Delta_{SDW} = -U \sum_k \langle C_{k\uparrow}^+ C_{k-Q\downarrow} \rangle \quad (1.5.2)$$

Frohlich considered a possible sliding of the collective state involving electrons and lattice displacements in the one dimensional metal as a manifestation of superconductivity. And the energy gap that emerge with this spectrum is identified to

be superconducting rather than dielectric peierls gap. However the discovery of high conductivity in organic salt TTF-TCNQ suggest that the coherent transport phenomena appropriate to quasi one dimensional substances to be a manifestation of a quite different collective state:  $CDW_s$  coupled with periodic lattice distortions [19].

At low temperature a quasi one dimensional metals become unstable for external perturbations with the wave number  $2k_F$ , where  $k_F$  is Fermi wave number. The  $2k_F$  modulated electronic structure corresponds to an electron density modulation, and hence is called a charge density wave(CDW). Since this structure is usually accompanied by a static lattice deformation of the same wave number through electron-phonon interaction, the CDW is regarded as a collective mode of coupled electron and lattice systems [12]. CDW state is coherent superposition of pairs of electrons and holes with parallel spin, but the pairs have opposite spin for SDW. Thus the CDW ground state is non magnetic, while that of SDW has well defined magnetic character. For both density waves, low lying charge excitations are related to spatial variations of the phase and are called phasons. The coupling mechanism which leads to CDW ground state is electron-phonon coupling, while the SDW state is due to electron-electron interaction.

Systems that exhibit  $CDW_s$  are typically quasi one-dimensional metals. They become insulator at the phase transition to CDW state. The periodicity nature of lattice deformation lead to the periodic electron density modulation. This modulation provide an energy gap in the single-particle excitation spectrum at the fermi level(1.2)b. In the system of non interacting electrons and phonons, the ions are equally spaced and charge density is uniform(1.2)a, while if the electrons and phonons are allowed to interact, the competition between elastic and electronic energies leads to a static

lattice deformation and periodically modulated charge density(1.2)b, which is called Peierls instability [20].

There are two kinds of CDW; one is the bond ordering wave in which the charge density is spatially modulated according to the distribution of bonding electrons, while the other is the charge ordering wave which is found in one-dimensional charge transfer salts, where charge density is determined from the distribution of conduction electrons [12]. The charge density associated with the collective mode is given by [16];

$$\rho(\mathbf{r}) = \rho_0 + \rho_1 \cos(2\mathbf{k}_F \cdot \mathbf{r} + \varphi) \quad (1.5.3)$$

where  $\rho_0$  is the unperturbed electron density of the metal.

## 1.6 Coexistence state

It is the formation of cooper pair from electrons of opposite spins and momenta that is responsible for superconductivity, while magnetism arise due to spin polarization. Thus, naturally one order would inhibit the other, means magnetism and superconductivity are mutually exclusive phenomenons. SDW result in condensation of electron-hole pairs of opposite spins but with a momentum difference of  $\mathbf{Q}$  between the conjugates, which is similar to the formation of superconductivity through condensation of electron-electron pairs. This leads to the instability of Fermi surface with respect to the set in(superconductivity or SDW) condensate state. This means if one phase sets in first and exists over all the Fermi surface, there will no possibility to the other phase, since no more carriers available to form pairs. But in reality the two phases coexist under different circumstances [17].

A number of interesting systems exhibit coexisting superconductivity and SDW order. The best example for this is the quasi one dimensional organic substance

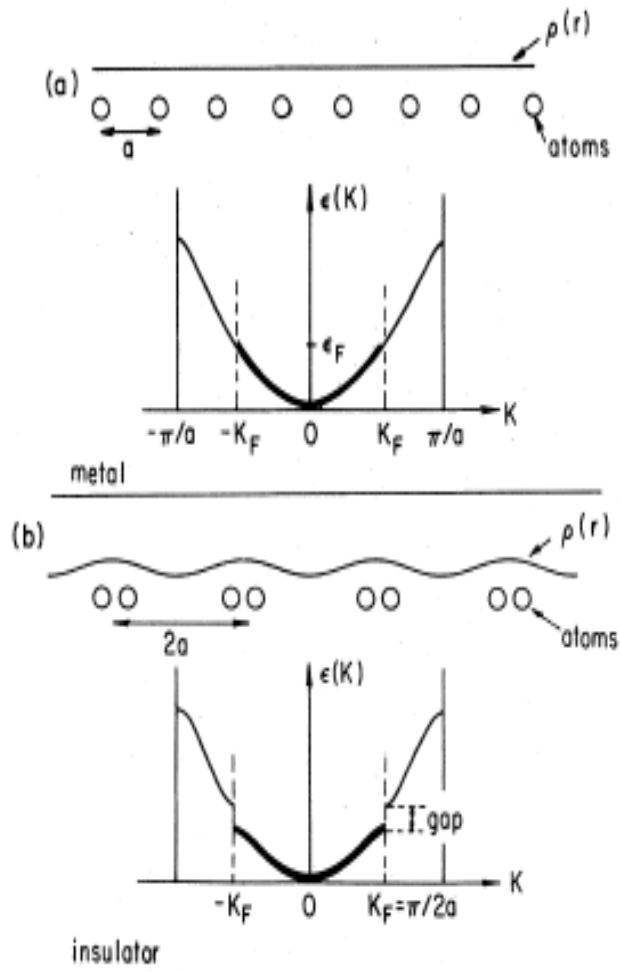


Figure 1.2: Peierls distortion in a one-dimensional metal with a half-filled band

$(TMTSF)_2ClO_4$ , which is one of the so-called Bechgaard salts with the general formula  $(TMTSF)_2X$ , where TMTSF is organic cation and X is an inorganic monoanion. These compounds are charge transfer salts which are formed by transferring one electron from two TMTSF molecules to one X. The first organic material which was discovered to show superconductivity was pressurized  $(TMTSF)_2PF_6$ .

Although, the electrical conduction in organic crystals began to draw the attention of scientists just after perylene bromine complex was found to display a marked increase in conductivity over other materials, primarily they have been regarded as electrical insulators. The organic metals are the richly varied organic charge transfer salts, the intermolecular compounds stabilized by the partial transfer of electrons between constituent molecules. In bechgaard family TMTSF molecules are stacked in columns along which the highest conductivity occurs. Then a considerable transverse coupling between the columns is crucial in realizing good metallic conductivity down to low temperatures and in impeding the appearance of an insulating phase, which has been recognized as been an SDW phase. This type of insulating state is suppressed by breaking the Fermi surface nesting by increasing or modulating the transverse intercolumnar coupling [12].

Quasi one-dimensional organic compounds of the  $(TM)_2X$ , where TM is either TMTTF or TMTSF, family can be described by a unified pressure-temperature(P-T) phase diagram. SDW and superconductivity compete in the region of high pressure and low temperature, while low pressure and high temperature region characterized by Mott-Hubbard localization. In P-T phase diagram of  $(TMTSF)_2PF_6$  superconductivity and SDW phase coexist below a temperature  $T_c = 1.20 \pm 0.01k$  [21] with

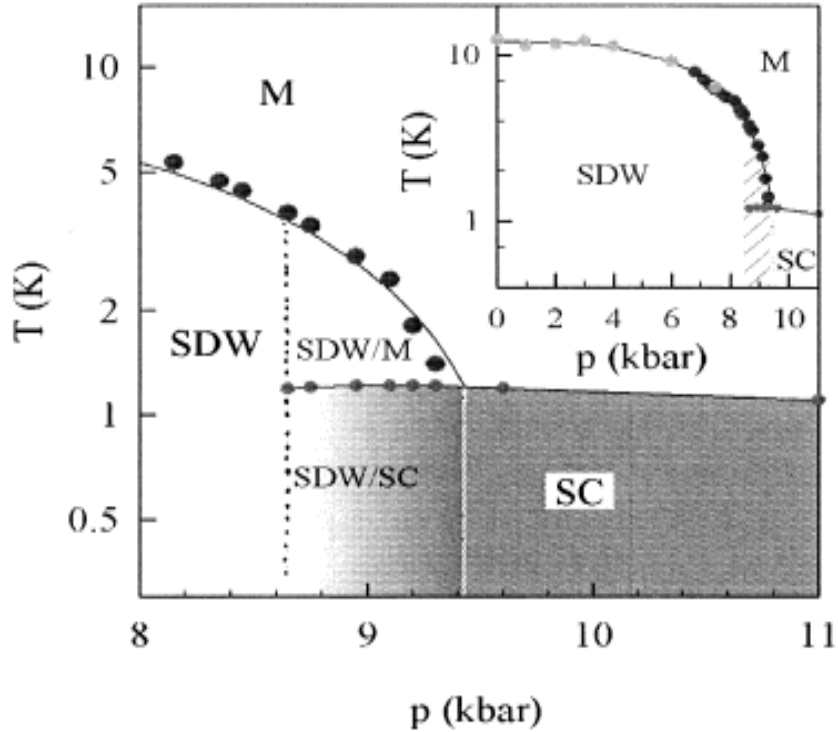


Figure 1.3: Pressure temperature phase diagram of  $(TMTSF)_2PF_6$  in the 8-11kbar range

in a narrow pressure range 8.6-9.4kbar as shown in Fig(1.3). This compound undergoes metal-SDW insulator transition near 12k at ambient pressure due to nesting of the Fermi surface, but one can worsen the Fermi surface nesting condition by applying a pressure above 6kbar and recover the metallic phase [22]. The experiment clearly demonstrates that in real three dimension, although anisotropic, materials in the superconducting and electron-hole pairings do coexist in a robust manner, which suggests that coexistence is not a peculiar character of one dimensional metals [19].

Metal-insulator transition will be induced by isotropic SDW on the perfectly nesting Fermi surface, where the entire Fermi surface could be isotropically gaped. If the

system is doped with holes or electrons removed from the valence SDW band, the Fermi surface perfect nesting will be deviated leading to suppression of SDW gap, which act as a potential well for the injected hole in which it gets self trapped to form "spin bag". Two holes can dig a deeper well and stay together with opposite spins and can be considered as cooper pairs. And coherent movement of such bags result in superconductivity. Hence superconductivity can arise over the isotropic SDW state for very small hole concentration.

SDW show anisotropic character when a system have nested pieces of Fermi surface only in certain direction and no nesting in other direction. This anisotropy will result due to peculiar topology of the Fermi surface or due to large doping of the system. In the regions of the Fermi surface where SDW gap vanishes or SDW state is completely suppressed(i.e., where nesting destroyed), the SDW quasi particles can interact with each other and form pairs leading to superconductivity, which is fundamentally different from the origin of conventional superconductivity [17].

For most superconductors, suspected or shown to undergo another transition of the spin singlet(CDW) or spin triplet(SDW) type, the main question is weather the gapping of the Fermi surface is favorable or destructive of superconductivity rather than about the coexistence of cooper and electron-hole pairings, because the later can be proved experimentally with relative ease. Here there are two contradicting concepts: gapping was demonstrated to cause detrimental effect on superconductivity [ref.19], and the superconducting critical temperature,  $T_c$ , is enhanced by the singular electron density of states near the dielectric gap edge [23]. Since superconductivity is found to weakly compete in the struggle of the Fermi surface, the better way of enhancing  $T_c$  is to avoid SDW/CDW gap. However it is necessary to mention the stimulation

of d-wave or even p-wave superconductivity by CDW/SDW induced reconstruction of the electron spectrum [24] or by renormalization of the electron-electron interaction due to a static incommensurate CDW background [25]. Moreover the possible coexistence of CDW and SDW was proved by different theoreticians [26].

# Chapter 2

## Mathematical Techniques

### 2.1 Introduction

One of the main ingredients in BCS theory is an effective attractive interaction between two electrons that have opposite momenta (larger in magnitude than the Fermi momentum) and opposite spins which leads to the formation of the Cooper pairs, which inturn condensate in to a single coherent quantum state called the "superconducting condensate" which is responsible for all superconducting phenomena. The effective electron-electron interaction term is derived in the next section. Moreover, a brief introduction about Green's function, which will be used entirely in the next chapter to manipulate the problem, is given in this chapter.

### 2.2 Effective Electron-Electron Interaction

Interaction between two electrons in a solid separated by a distance  $\mathbf{r}$  in real space is given by bare coulomb potential (assuming that the ions are fixed in space);

$$V(\mathbf{r}) = \frac{e^2}{|\mathbf{r}|}$$

This interaction can be considered as scattering process corresponding to the exchange of photons with wavevector  $\mathbf{q}$ . But, in the solid, it is screened by all the other electrons and the screening effect is included in Yukawa potential as;

$$V(\mathbf{r}) = \frac{e^2 e^{-k_s |\mathbf{r}|}}{|\mathbf{r}|}$$

where  $k_s$  is the inverse screening length [9]. The Fourier transformation of this equation is given by;

$$V(\mathbf{q}) = \frac{4\pi e^2}{|\mathbf{q}|^2 + k_s^2}$$

where  $\mathbf{q}$  is the momentum of photon that involved in the scattering process.

When the ions in a solid are allowed to move, the interaction term given above will be changed. The positively charged ions will be attracted by an electron that moves through the solid, as it approaches and retain their equilibrium position slowly following the electron has passed them by, and this motion can be related to phonons emitted by the traveling electron. The collective motion of ions toward one electron leads to attractive interaction between other electrons and the traveling electron because the electrons themselves are attracted to the ions.

Due to this attractive interaction between two electrons near the Fermi surface, caused by their interaction with the zero point phonon, the so called Cooper pairs are formed. And this is the interaction that is responsible for superconducting phenomena in elements which exhibit isotope effect. In this section we discuss this effective electron-electron interaction caused by electron-phonon interaction. The total Hamiltonian for electron-phonon interaction of the deformation-potential type in ordinary

superconductors is given by [27];

$$\begin{aligned} H &= H_0 + H' \\ &= \sum_k \varepsilon_{\mathbf{k}} c_k^\dagger c_k + \sum_q \omega_q a_q^\dagger a_q + \imath g \sum_{k,q} c_{k+q}^\dagger c_k (a_q - a_{-q}^\dagger) \end{aligned} \quad (2.2.1)$$

Where  $(c^+, c)$  are fermion operators while  $(a^+, a)$  are boson operators and  $g$  is electron-phonon interaction constant.  $H_0$  represent the hamiltonian of free electrons and phonons while  $H'$  stands for coupling interaction. But in first order the interaction term,  $H'$ , leads to electron scattering and coupling will result in the second order. Hence to eliminate the first order term from the hamiltonian and to extract an effective electron-electron interaction from the electron-phonon interaction we shall make a canonical transformation;

$$\tilde{H} = e^{-S} H e^S \quad (2.2.2)$$

Where  $S$  is an antiunitary operator, i.e.  $S^\dagger = -S$ , such that  $e^S$  is unitary. By performing a unitary transformation, all physical quantities remain unchanged. And in the interaction picture  $S$  can be given by;

$$S_I(t) = -i\lambda \int_{-\infty}^t dt' H_I'(t')$$

Then by using power series equation (2.2.1) can be written as;

$$\begin{aligned} \tilde{H} &= (1 - S + \frac{1}{2}S^2 - \dots)H(1 + S + \frac{1}{2}S^2 + \dots) \\ &= H + [H, S] + \frac{1}{2}[[H, S], S] + \dots \end{aligned} \quad (2.2.3)$$

By taking  $H = H_0 + \lambda H'$  equation (2.2.3) can be written as;

$$\tilde{H} = H_0 + \lambda H' + [H_0, S] + [\lambda H', S] + \frac{1}{2}[[H_0, S], S] + \frac{1}{2}[[\lambda H', S], S] + \dots \quad (2.2.4)$$

We can chose S in such a way as to satisfy the following equation;

$$\lambda H' + [H_0, S] = 0 \quad (2.2.5)$$

$$SH_0 - H_0S = \lambda H'$$

$$\langle n | SH_0 | m \rangle - \langle n | H_0S | m \rangle = \langle n | \lambda H' | m \rangle$$

If we have eigen values  $E_m$  and  $E_n$ , for eigen states  $| m \rangle$  and  $| n \rangle$  respectively, i.e.,  $H_0 | n \rangle = E_n | n \rangle$  and  $H_0 | m \rangle = E_m | m \rangle$ , the above equation can be written as;

$$(E_m - E_n) \langle n | S | m \rangle = \lambda \langle n | H' | m \rangle$$

$$\langle n | S | m \rangle = \frac{\lambda \langle n | H' | m \rangle}{E_m - E_n} \quad (2.2.6)$$

provided that  $E_m \neq E_n$ . With the help of equation(2.2.5) equation (2.2.4) can be rewritten as;

$$\begin{aligned} \tilde{H} &= H_0 + \lambda[H', S] + \frac{1}{2}[[H_0, S], S] + \frac{1}{2}[[\lambda H', S], S] + \dots \\ &= H_0 + \lambda[H', S] + \frac{1}{2}[-\lambda H', S] + O(\lambda^3) \\ &= H_0 + \frac{1}{2}\lambda[H', S] + O(\lambda^3) \end{aligned} \quad (2.2.7)$$

Equation (2.2.5) suggest that S is in the order of  $\lambda$ ,  $S \sim \lambda$ , which inturn leads us to conclude that the transformed Hamiltonian does not involve a term which is linear in  $\lambda$ . To obtain effective electron-electron coupling we shall take the matrix element over the phonon operators leaving the fermion operators to be displayed explicitly. At absolute zero either of the eigen states,  $| n \rangle$  or  $| m \rangle$ , refers vacuum phonon states. If  $| 0 \rangle$  refers ground state while  $| 1_{\mathbf{q}} \rangle$  stands for excited state, and having the following relation for phonon creation and annihilation operators;

$$\langle m | a^+ + a | n \rangle = \sqrt{n+1}\delta_{m,n+1} + \sqrt{n}\delta_{m,n-1} \quad (2.2.8)$$

Then for an electron scattered from  $|0\rangle$  state to  $|1_{\mathbf{q}}\rangle$  state by creating a phonon we can write the following relation by involving only phonon creation operator;

$$\begin{aligned}
\langle 1_{\mathbf{q}} | S | 0 \rangle &= -ig \frac{\langle 1_{\mathbf{q}} | \sum_{\mathbf{kq}} c_{\mathbf{k+q}}^+ c_{\mathbf{k}} a_{-\mathbf{q}}^+ | 0 \rangle}{E_m - E_n} \\
&= -ig \frac{\sum_{\mathbf{kq}} c_{\mathbf{k+q}}^+ c_{\mathbf{k}} \langle 1_{\mathbf{q}} | a_{-\mathbf{q}}^+ | 0 \rangle}{E_0 - E_{1_{\mathbf{q}}}} \\
&= -ig \frac{\sum_{\mathbf{kq}} c_{\mathbf{k+q}}^+ c_{\mathbf{k}} \delta_{1,1} \sqrt{0+1}}{\varepsilon_{\mathbf{k}} - (\varepsilon_{\mathbf{k-q}} + \hbar\omega_{\mathbf{q}})} \\
&= -ig \sum_{\mathbf{k}} c_{\mathbf{k-q}}^+ c_{\mathbf{k}} \frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k-q}} - \hbar\omega_{\mathbf{q}}} \quad (2.2.9)
\end{aligned}$$

Similarly for an electron scattered from  $|1_{\mathbf{q}}\rangle$  to  $|0\rangle$  state by absorbing a phonon we can write the following equation in which only phonon annihilation operator is involved;

$$\begin{aligned}
\langle 0 | S | 1_{\mathbf{q}} \rangle &= ig \frac{\langle 0 | \sum_{\mathbf{k,q}} c_{\mathbf{k+q}}^+ c_{\mathbf{k}} a_{\mathbf{q}} | 1_{\mathbf{q}} \rangle}{E_{1_{\mathbf{q}}} - E_0} \\
&= ig \sum_{\mathbf{k}'} c_{\mathbf{k'+q}}^+ c_{\mathbf{k}'} \frac{1}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k'+q}} + \hbar\omega_{\mathbf{q}}} \quad (2.2.10)
\end{aligned}$$

Neglecting third and higher order in  $\lambda$  from equation (2.2.7) gives us;

$$\tilde{H} = H_0 + \frac{1}{2}\lambda[H', S] \quad (2.2.11)$$

We need now to perform the commutation  $[H', S]$ . To do this it is better to evaluate  $H'S$  and  $SH'$  independently.

$$\begin{aligned}
\langle n | H'S | m \rangle &= \sum_l \langle n | H' | l \rangle \langle l | S | m \rangle \\
&= \lambda \sum_l \langle n | H' | l \rangle \frac{\langle l | H' | m \rangle}{E_m - E_l} \quad (2.2.12)
\end{aligned}$$

If we restrict the states we are considering to be zero-phonon states, then for a particular phonon mode, equation (2.2.12) will become;

$$\langle n | H'S | m \rangle = \langle 0 | H' | 1_{\mathbf{q}} \rangle \frac{\langle 1_{\mathbf{q}} | H' | 0 \rangle}{E_m - E_l} \quad (2.2.13)$$

By taking the expression of  $H'$  from equation (2.2.1) and involving only phonon creation operator for scattering from  $|0\rangle$  to  $|1_q\rangle$  and phonon annihilation operator for scattering from  $|1_q\rangle$  to  $|0\rangle$  we will get the following expressions;

$$\begin{aligned} \langle 1_q | H' | 0 \rangle &= \langle 1_q | ig \sum_{\mathbf{k}, \mathbf{q}} c_{\mathbf{k}+\mathbf{q}}^+ c_{\mathbf{k}} (-a_{-\mathbf{q}}^+) | 0 \rangle \\ &= -ig \sum_{\mathbf{k}, \mathbf{q}} c_{\mathbf{k}-\mathbf{q}}^+ c_{\mathbf{k}} \end{aligned} \quad (2.2.14)$$

$$\begin{aligned} \langle 0 | H' | 1_q \rangle &= \langle 0 | ig \sum_{\mathbf{k}', \mathbf{q}} c_{\mathbf{k}'+\mathbf{q}}^+ c_{\mathbf{k}'} (a_{\mathbf{q}}) | 1_q \rangle \\ &= ig \sum_{\mathbf{k}', \mathbf{q}} c_{\mathbf{k}'+\mathbf{q}}^+ c_{\mathbf{k}'} \end{aligned} \quad (2.2.15)$$

Thus using equations (2.2.14) and (2.2.15), equation (2.2.13) can be given by;

$$\langle n | H' S | m \rangle = g^2 \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} c_{\mathbf{k}'+\mathbf{q}}^+ c_{\mathbf{k}'} c_{\mathbf{k}-\mathbf{q}}^+ c_{\mathbf{k}} \frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}} - \hbar\omega_{\mathbf{q}}} \quad (2.2.16)$$

Similarly we can solve for  $SH'$  ;

$$\begin{aligned} \langle n | SH' | m \rangle &= \lambda \sum_l \frac{\langle n | H' | l \rangle}{E_l - E_n} \langle l | H' | m \rangle \\ &= g^2 \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} c_{\mathbf{k}'+\mathbf{q}}^+ c_{\mathbf{k}'} c_{\mathbf{k}-\mathbf{q}}^+ c_{\mathbf{k}} \frac{1}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}'-\mathbf{q}} + \hbar\omega_{\mathbf{q}}} \end{aligned} \quad (2.2.17)$$

Then with the help of equations (2.2.16) and (2.2.17) equation (2.2.11) can be rewritten as;

$$\tilde{H} = H_0 + \frac{1}{2} g^2 \sum_{\mathbf{q}, \mathbf{k}, \mathbf{k}'} c_{\mathbf{k}'+\mathbf{q}}^+ c_{\mathbf{k}'} c_{\mathbf{k}-\mathbf{q}}^+ c_{\mathbf{k}} \left( \frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}} - \hbar\omega_{\mathbf{q}}} - \frac{1}{\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}'-\mathbf{q}} + \hbar\omega_{\mathbf{q}}} \right) \quad (2.2.18)$$

After summing over the terms in  $\mathbf{q}$  and  $-\mathbf{q}$  with the approximation  $\omega_{\mathbf{q}} = \omega_{-\mathbf{q}}$  we will get;

$$\tilde{H} = H_0 + \frac{1}{4} g^2 \sum_{\mathbf{k}, \mathbf{k}'} c_{\mathbf{k}'+\mathbf{q}}^+ c_{\mathbf{k}'} c_{\mathbf{k}-\mathbf{q}}^+ c_{\mathbf{k}} \frac{4\hbar\omega_{\mathbf{q}}}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})^2 - (\hbar\omega_{\mathbf{q}})^2} \quad (2.2.19)$$

But the interaction can be attractive only in the vicinity of the fermi surface where energy difference of the two interacting electrons is less than the phonon energy,  $|\varepsilon_{\mathbf{k}\pm\mathbf{q}} - \varepsilon_{\mathbf{k}}| < \hbar\omega_{\mathbf{q}}$ , and coulomb repulsion is dominated by phonon interaction for sufficiently large interaction constant  $g$ , which is possible with in the range  $\varepsilon_F - \hbar\omega_D < \varepsilon_{\mathbf{k}}$  and  $\varepsilon_{\mathbf{k}\pm\mathbf{q}} < \varepsilon_F + \hbar\omega_D$ . Thus equation (2.2.19) will be reduced to;

$$\tilde{H} = H_0 - V \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} c_{\mathbf{k}+\mathbf{q}}^+ c_{\mathbf{k}} c_{\mathbf{k}'-\mathbf{q}}^+ c_{\mathbf{k}'} \quad (2.2.20)$$

Where the interaction constant  $V$  takes the value roughly  $\frac{g^2}{\hbar\omega_{\mathbf{q}}}$ . And then, generally, equation (2.2.20) can be written as;

$$\tilde{H} = \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^+ c_{\mathbf{k}, \sigma} - V \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} c_{\mathbf{k}+\mathbf{q}\uparrow}^+ c_{\mathbf{k}\uparrow} c_{\mathbf{k}'-\mathbf{q}\downarrow}^+ c_{\mathbf{k}'\downarrow} \quad (2.2.21)$$

Which, in the mean field approximation, can be written as;

$$\tilde{H} = \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^+ c_{\mathbf{k}, \sigma} + \Delta_{sc} \sum_{\mathbf{k}} (c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}) \quad (2.2.22)$$

where;

$$\Delta_{SC} = -V \sum_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ \rangle$$

## 2.3 Green's Function

One of the most successful approaches to the many body problem is the canonical transformation technique. 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 problem. To deal with the many body problem, first one need to express the Hamiltonian of a system in terms of creation and annihilation operators. Recently the so-called Green's function became very popular way to solve statistical

problems in quantum field theory and sometimes they are called propagators because physical properties of a given system can be discussed based on the average behavior of only one or two typical particles, which are characterized by one-particle and two-particle propagators respectively. The popularity of Green's function becomes from its advantage of directness and flexibility. In many body problem Green's function is sometimes also called correlation function referring to correlators of field operators or creation and annihilation operators.

A Green's function is an integral kernel that can be used to solve an inhomogeneous differential equation with boundary conditions. This concept was first developed by British mathematician George Green in 1830, and this is why the function is named after him. And it is used in physics to refer to various types of correlation functions. For an arbitrary linear differential operator  $\tilde{T}$  in three dimensions, the Green's function  $G(\mathbf{r}, \mathbf{r}')$  can be defined as;

$$\tilde{T}G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$$

Green's functions play an important role in the solution of linear ordinary and partial differential equations, and are a key component to the development of boundary integral equation methods. There are different types of Green's functions; one-particle, two-particle, ..., n-particle, advanced, retarded, casual, zero temperature, finite-temperature, real-time, imaginary-time, etc. But in this work we use double-time temperature-dependent Green's function.

Before discussing it we shall see the general properties of Green's function by accomplishing single-particle Green's function. If a particle with momentum  $\mathbf{k}$  is added to the ground state  $|\psi_0\rangle$  at, time  $t = 0$ , then the system will be described by  $c_{\mathbf{k}}^+ |\psi_0\rangle$  and its development with time is given by  $\exp(-\frac{iHt}{\hbar})c_{\mathbf{k}}^+ |\psi_0\rangle$ , where  $c_{\mathbf{k}}^+$  is

creation operator. Since at time  $t$  the ground state is described by  $\exp(-\frac{iHt}{\hbar}) | \psi_0 \rangle$  the probability amplitude for the persistence of the added particle in the precise momentum state  $\mathbf{k}$  at time  $t$  is given by  $\langle \psi_0 | e^{\frac{iHt}{\hbar}} c_{\mathbf{k}} e^{-\frac{iHt}{\hbar}} c_{\mathbf{k}}^+ | \psi_0 \rangle$ . With this analogy single-particle Green's function can be defined as;

$$G(\mathbf{k}, t) = -i \langle \mathbf{k}, \mathbf{0} | \mathbf{k}, t \rangle; \quad \text{for } t > 0$$

which can be written in terms of creation and annihilation operator of an electron as;

$$\begin{aligned} G(\mathbf{k}, t) &= -i \langle 0 | c_{\mathbf{k}}(t) c_{\mathbf{k}}^+(0) | 0 \rangle \\ &= -i \sum_n \langle 0 | e^{iHt} c_{\mathbf{k}}(0) e^{-itH} | n \rangle \langle n | c_{\mathbf{k}}^+(0) | 0 \rangle \\ &= -i \sum_n \langle 0 | c_{\mathbf{k}} | n \rangle \langle n | c_{\mathbf{k}}^+ | 0 \rangle e^{-i\xi_n t} \\ &= -i \sum_n (|\langle n | c_{\mathbf{k}}^+ | 0 \rangle|^2) e^{-i\xi_n t}; \quad t > 0 \end{aligned}$$

where  $\xi_n = E_n(N+1) - E_n(N)$  and  $| 0 \rangle$  refers the vacuum state, and we take  $\hbar = 1$ .

Taking the Fourier transformation;

$$\begin{aligned} G(\mathbf{k}, \omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G(\mathbf{k}, t) \\ &= -i \int_{-\infty}^{\infty} dt \sum_n |\langle n | c_{\mathbf{k}}^+(0) | 0 \rangle|^2 e^{i(\omega - \xi_n)t} \\ &= \sum_n \frac{|\langle n | c_{\mathbf{k}}^+ | 0 \rangle|^2}{\omega - \xi_n + i\delta} \end{aligned} \tag{2.3.1}$$

where the positive infinitesimal delta appears to ensure that  $G(\mathbf{k}, t) = 0$  for  $t < 0$ .

Similarly hole Green function can be written as;

$$\begin{aligned} G(\mathbf{k}, t) &= i \langle 0 | c_{\mathbf{k}}^+(0) c_{\mathbf{k}}(t) | 0 \rangle; \quad t < 0 \\ G(\mathbf{k}, \omega) &= - \sum_n \frac{|\langle n | c_{\mathbf{k}}(0) | 0 \rangle|^2}{\omega - \xi_n - i\delta} \end{aligned} \tag{2.3.2}$$

Time-ordered or casual Green's function can be developed by combining equations(2.3.1) and(2.3.2);

$$G_c(\mathbf{k}, t) = -i \langle 0 | T(c_{\mathbf{k}}(t)c_{\mathbf{k}}(0)) | 0 \rangle$$

And the space-time Green's function can be defined by;

$$G(xt; x't') = -i \langle 0 | T(\psi(x, t)\psi^+(x't')) | 0 \rangle$$

where  $\psi(xt)$  is Heisenberg operator for the wave field and T is chronological operator which order earlier time to the right and simultaneously multiplies that on which it operates by  $(-1)^p$ , where p is the number of exchanges of fermion operators needed to accomplish the desired ordering.

### 2.3.1 Double-Time Temperature-Dependent Green's Function

Green's function in statistical mechanics are the appropriate generalizations of the correlation functions. The retarded and advanced Green's functions are defined as;

$$G_r(t, t') = \ll A(t); B(t') \gg_r = -i\theta(t - t') \langle [A(t), B(t')] \rangle \quad (2.3.3)$$

$$G_a(t, t') = \ll A(t); B(t') \gg_a = i\theta(t' - t) \langle [A(t), B(t')] \rangle \quad (2.3.4)$$

where  $\ll \dots \gg$  represents the Green's function,  $\theta(t - t')$  is heviside step function. The Heaviside step function,  $\theta(t - t')$ , also called unit step function, is a discontinuous function whose value is zero for negative argument and one for positive argument. The Heaviside function is an antiderivative of the Dirac delta function

$$\theta(t - t') = \int_{-\infty}^t \delta(t) dt$$

And  $\langle \dots \rangle$  denotes averaging over a grand canonical ensemble which can be defined as ;

$$\begin{aligned}\langle \dots \rangle &= Z^{-1} \text{Tr}(e^{-\beta H} \dots) \\ Z &= \text{Tr}(e^{-\beta \Omega})\end{aligned}$$

where  $Z$  is the grand partition function,  $\Omega$  is the thermodynamic potential, and  $H$  is the Hamiltonian of the system considered.  $A(t)$  and  $B(t')$  are operators in the Heisenberg representation and can be expressed as;

$$A(t) = \exp(iHt)A(0)\exp(-iHt) \quad (2.3.5)$$

$[A(t), B(t')]$  stands for commutation or anticommutation;

$$[A(t), B(t')] = A(t)B(t') - \eta B(t')A(t)$$

with  $\eta = +1$  for bose operators and  $\eta = -1$  for fermi operators.

$$G_r(t, t') = -i\theta(t - t')[\langle A(t)B(t') \rangle - \eta \langle B(t')A(t) \rangle]$$

Where the Heviside step function have magnitude;

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

Thus  $G_r(t, t') \neq 0$  for  $t' < t$ ,  $G_r(t, t') = 0$  for  $t' > t$ , and it is undefined for  $t' = t$  because of the discontinuity of heviside step function  $\theta(t)$  at  $t = 0$ . Using equation(2.3.5) we can write;

$$\begin{aligned}A(t)B(t') &= e^{iHt}A(0)e^{-iHt}e^{iHt'}B(0)e^{-iHt'} \\ &= e^{iHt}e^{-iHt'}A(0)e^{-iHt}e^{iHt'}B(0)e^{-iHt'}e^{iHt'} \\ &= e^{iH(t-t')}A(0)e^{-iH(t-t')}B(0)\end{aligned}$$

Similarly

$$B(t')A(t) = e^{\imath H(t'-t)}B(0)e^{-\imath H(t'-t)}A(0) \quad (2.3.6)$$

With these we can write;

$$\begin{aligned} G_r(t, t') &= - \imath \theta(t - t') [\langle A(t)B(t') \rangle - \eta \langle B(t')A(t) \rangle] \\ &= - \imath \theta(t - t') \langle A(t)B(t') \rangle - \imath \eta \theta(t' - t) \langle B(t')A(t) \rangle \\ &= - \imath \theta(t - t') \text{Tr}(e^{-\beta H} A(t)B(t')) - \imath \eta \theta(t' - t) \text{Tr}(e^{-\beta H} B(t')A(t)) \\ &= - \imath \theta(t - t') \text{Tr}[e^{H[\imath(t-t')-\beta]} A(0)e^{-\imath H(t-t')} B(0)] \\ &\quad - \imath \eta \theta(t' - t) \text{Tr}[e^{H[\imath(t'-t)-\beta]} B(0)e^{-\imath H(t'-t)} A(0)] \\ &= G_r(t - t') \end{aligned} \quad (2.3.7)$$

Thus both green's functions and time correlation functions  $\langle A(t)B(t') \rangle$  and  $\langle B(t')A(t) \rangle$  depend only on the difference  $(t - t')$ . By differentiating the retarded Green's function we can solve the equation of motion as follows;

$$\begin{aligned} \imath \frac{dG}{dt} &= \imath \frac{d}{dt} \lll A(t)B(t') \ggg \\ &= \frac{d}{dt} \theta(t - t') \langle [A(t)B(t')] \rangle \\ &= \frac{d}{dt} [\theta(t - t') \langle A(t)B(t') - \eta B(t')A(t) \rangle] \\ &= \frac{d}{dt} \theta(t - t') \langle [A(t)B(t')] \rangle + \theta(t - t') \langle \left[ \frac{d}{dt} A(t), B(t') \right] \rangle \\ &= \frac{d}{dt} \theta(t - t') \langle [A(t)B(t')] \rangle + \lll \imath \frac{d}{dt} A(t), B(t') \ggg \\ &= \frac{d}{dt} \theta(t - t') \langle [A(t)B(t')] \rangle + \lll [A(t), H], B(t') \ggg \end{aligned} \quad (2.3.8)$$

Using a relation  $\theta(t - t') = \int_{-\infty}^t \delta(t-t') dt \implies \frac{d}{dt} \theta(t - t') = \delta(t - t')$  we can write;

$$\begin{aligned} \imath \frac{dG}{dt} &= \delta(t - t') \langle [A(t)B(t')] \rangle + \lll [A(t), H], B(t') \ggg \\ &= \langle [A(t)B(t')] \rangle + \lll [A(t), H], B(t') \ggg \quad \text{for } t > t' \end{aligned} \quad (2.3.9)$$

The Fourier transformation of the Green's function can be written as;

$$G_{AB}(t, t') = \int G(\omega) e^{-i\omega(t-t')} d\omega$$

Thus after differentiation we can have;

$$\begin{aligned} \frac{dG}{dt} &= -i\omega \int G(\omega) e^{-i\omega(t-t')} d\omega \\ &= -i\omega \times \text{fourier transform of } G(t) \end{aligned}$$

Finally equation(2.3.9) can be written as;

$$\omega \ll A(t), B(t') \gg_{\omega} = \langle [A(t)B(t')] \rangle + \ll [A(t), H], B(t') \gg_{\omega} \quad (2.3.10)$$

# Chapter 3

## Mathematical Formulation Of The Problem

### 3.1 Coexistence Of SDW and Singlet Superconductivity

In non triplet systems local AF order and singlet superconductivity(SS) can in principle coexist since AF order favors singlet correlations [5]. We can adopt the Hamiltonian for coexistence state from those of each independent states(Sc and SDW states), i.e., from equations (1.2.1) and (1.5.1) by adding the interaction term on SDW hamiltonian, and then in the mean field approximation it can be written as;

$$H = \sum_{p,\sigma} \varepsilon_p C_{p\sigma}^+ C_{p\sigma} + \Delta_{SDW} \sum_p (C_{p+Q\uparrow}^+ C_{p\downarrow} + C_{p\downarrow}^+ C_{p+Q\uparrow}) + \Delta_{SC} \sum_p (C_{p\uparrow}^+ C_{-p\downarrow}^+ + C_{-p\downarrow} C_{p\uparrow}) \quad (3.1.1)$$

where a SDW order parameter,  $\Delta_{SDW}$ , is given by:

$$\Delta_{SDW} = -U \sum_k \langle C_{k\uparrow}^+ C_{k-Q\downarrow} \rangle \quad (3.1.2)$$

While the superconducting order parameter,  $\Delta_{SC}$ , is given by;

$$\Delta_{SC} = -V \sum_k \langle C_{-k\downarrow} C_{k\uparrow} \rangle = -V \sum_k \langle C_{k\uparrow}^+ C_{-k\downarrow}^+ \rangle \quad (3.1.3)$$

Where we have made the assumption that the order parameter is real,  $\Delta_{SC} = \Delta_{sc}^*$ .

### 3.1.1 The order parameter of SDW

The order parameter of SDW is given by equation (3.1.2). Thus, using Green's function, the equation of motion for the correlation can be written as;

$$\begin{aligned} \omega \ll c_{k\uparrow}^+ c_{k-Q\downarrow} \gg &= \langle \{C_{k\uparrow}^+, C_{k-Q\downarrow}\} \rangle + \ll [C_{k\uparrow}^+, H], C_{k-Q\downarrow} \gg \\ &= \ll [C_{k\uparrow}^+, H], C_{k-Q\downarrow} \gg \end{aligned} \quad (3.1.4)$$

To solve this equation of motion first we have to calculate the commutation relation which appears in the right hand side(RHS) of equation (3.1.4). And it is done in the following way;

$$\begin{aligned} [C_{k\uparrow}^+, H] &= \sum_{p\sigma} \varepsilon_p [C_{k\uparrow}^+, C_{p\sigma}^+ C_{p\sigma}] + \Delta_{SDW} \sum_p [C_{k\uparrow}^+, C_{p+Q\uparrow}^+ C_{p\downarrow}] + [C_{k\uparrow}^+, C_{p\downarrow}^+ C_{p+Q\uparrow}] \\ &+ \Delta_{SC} \sum_p [C_{k\uparrow}^+, C_{p\uparrow}^+ C_{-p\downarrow}] + [C_{k\uparrow}^+, C_{-p\downarrow} C_{p\uparrow}] \end{aligned} \quad (3.1.5)$$

$$\begin{aligned} [C_{k\uparrow}^+, H] &= \sum_{p\sigma} \varepsilon_p \{C_{k\uparrow}^+ C_{p\sigma}^+\} C_{p\sigma} - C_{p\sigma}^+ \{C_{k\uparrow}^+ C_{p\sigma}\} \\ &+ \Delta_{SDW} \sum_p \{C_{k\uparrow}^+ C_{p+Q\uparrow}^+\} C_{p\downarrow} - C_{p+Q\uparrow}^+ \{C_{k\uparrow}^+ C_{p\downarrow}\} + \{C_{k\uparrow}^+ C_{p\downarrow}^+\} C_{p+Q\uparrow} - C_{p\downarrow}^+ \{C_{k\uparrow}^+ C_{p+Q\uparrow}\} \\ &+ \Delta_{SC} \sum_p \{C_{k\uparrow}^+ C_{p\uparrow}^+\} C_{-p\downarrow} - C_{p\downarrow}^+ \{C_{k\uparrow}^+ C_{-p\downarrow}\} + \{C_{k\uparrow}^+ C_{-p\downarrow}\} C_{p\uparrow} - C_{-p\downarrow} \{C_{k\uparrow}^+ C_{p\downarrow}\} \end{aligned} \quad (3.1.6)$$

Where we have used the property;

$$[A, BC] = \{A, B\}C - B\{A, C\} \quad (3.1.7)$$

which is valid for any fermion operators A, B, and C, because fermion operators, unlike boson operators, satisfy anticommutation relation rather than commutation relation. Then by using anticommutation relation

$$\{C_{k\sigma}^+ C_{k'\sigma'}\} = \delta_{k,k'} \delta_{\sigma,\sigma'}; \{C_{k\sigma}^+ C_{k'\sigma'}^+\} = \{C_{k\sigma} C_{k'\sigma'}\} = 0 \quad (3.1.8)$$

equation(3.1.6) becomes;

$$\begin{aligned} [C_{k\uparrow}^+, H] &= \sum_{p\sigma} -\varepsilon_p C_{p\sigma}^+ \{C_{k\uparrow}^+ C_{p\sigma}\} + \Delta_{SDW} \sum_p -C_{p\downarrow}^+ \{C_{k\uparrow}^+ C_{p+Q\uparrow}\} + \Delta_{SC} \sum_p -C_{-p\downarrow} \{C_{k\uparrow}^+ C_{p\uparrow}\} \\ &= -\sum_{p\sigma} \varepsilon_p C_{p\sigma}^+ \delta_{k,p} \delta_{\uparrow\sigma} - \Delta_{SDW} \sum_p C_{p\downarrow}^+ \delta_{k,p+Q} - \Delta_{SC} \sum_P C_{-P\downarrow} \delta_{k,p} \\ &= -\varepsilon_k C_{k\uparrow}^+ - \Delta_{SDW} C_{k-Q\downarrow}^+ - \Delta_{SC} C_{-k\downarrow} \end{aligned} \quad (3.1.9)$$

$$\omega \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = -\varepsilon_k \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg - \Delta_{SDW} \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg - \Delta_{SC} \ll C_{-k\downarrow} C_{k-Q\downarrow} \gg \quad (3.1.10)$$

$$(\omega + \varepsilon_k) \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = -\Delta_{SDW} \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg - \Delta_{SC} \ll C_{-k\downarrow} C_{k-Q\downarrow} \gg \quad (3.1.11)$$

The equation of motion for the first correlation in RHS of equation (3.1.11) can be written as;

$$\begin{aligned} \omega \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg &= \langle \{C_{k-Q\downarrow}^+, C_{k-Q\downarrow}\} \rangle + \ll [C_{k-Q\downarrow}^+, H], C_{k-Q\downarrow} \gg \\ &= 1 + \ll [C_{k-Q\downarrow}^+, H], C_{k-Q\downarrow} \gg \end{aligned} \quad (3.1.12)$$

Similarly we can write;

$$[C_{k-Q\downarrow}^+, H] = -\varepsilon_{k-Q} C_{k-Q\downarrow}^+ - \Delta_{SDW} C_{k\uparrow}^+ + \Delta_{SC} C_{-k+Q\uparrow} \quad (3.1.13)$$

Then, by inserting equation (3.1.13) in equation (3.1.12) we can get;

$$(\omega + \varepsilon_{k-Q}) \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg = 1 - \Delta_{SDW} \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg + \Delta_{SC} \ll C_{-k+Q\uparrow} C_{k-Q\downarrow} \gg \quad (3.1.14)$$

The equation of motion for the last correlation in RHS of(3.1.14) is;

$$\begin{aligned}\omega \ll C_{-k+Q\uparrow} C_{k-Q\downarrow} \gg &= \langle \{C_{-k+Q\uparrow} C_{k-Q\downarrow}\} \rangle + \ll [C_{-k+Q\uparrow}, H], C_{k-Q\downarrow} \gg \\ &= \ll [C_{-k+Q\uparrow}, H], C_{k-Q\downarrow} \gg\end{aligned}\quad (3.1.15)$$

Similarly solving the commutation relation gives us;

$$[C_{-k+Q\uparrow}, H] = \varepsilon_{-k+Q} C_{-k+Q\uparrow} + \Delta_{SDW} C_{-k\downarrow} + \Delta_{SC} C_{k-Q\downarrow}^+ \quad (3.1.16)$$

Thus using equation (3.1.16) in equation (3.1.15) we will get;

$$(\omega - \varepsilon_{-k+Q}) \ll C_{-k+Q\uparrow} C_{k-Q\downarrow} \gg = \Delta_{SDW} \ll C_{-k\downarrow} C_{k-Q\downarrow} \gg + \Delta_{SC} \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg \quad (3.1.17)$$

Still writing the equation of motion for the first correlation in equation(3.1.17) gives as;

$$\begin{aligned}\omega \ll C_{-k\downarrow} C_{k-Q\downarrow} \gg &= \langle \{C_{-k\downarrow} C_{k-Q\downarrow}\} \rangle + \ll [C_{-k\downarrow}, H], C_{k-Q\downarrow} \gg \\ &= \ll [C_{-k\downarrow}, H], C_{k-Q\downarrow} \gg\end{aligned}\quad (3.1.18)$$

$$(\omega - \varepsilon_{-k}) \ll C_{-k\downarrow} C_{k-Q\downarrow} \gg = \Delta_{SDW} \ll C_{-k+Q\uparrow} C_{k-Q\downarrow} \gg - \Delta_{SC} \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg \quad (3.1.19)$$

Using equations (3.1.14) and (3.1.19) in equation (3.1.11) gives us;

$$\begin{aligned}(\omega + \varepsilon_k) \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg &= -\frac{\Delta_{SDW}}{\omega + \varepsilon_{k-Q}} [1 - \Delta_{SDW} \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg + \Delta_{SC} \ll C_{-k+Q\uparrow} C_{k-Q\downarrow} \gg] \\ &\quad - \frac{\Delta_{SC}}{\omega - \varepsilon_{-k}} [\Delta_{SDW} \ll C_{-k+Q\uparrow} C_{k-Q\downarrow} \gg - \Delta_{SC} \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg] \quad (3.1.20)\end{aligned}$$

$$\begin{aligned}[(\omega + \varepsilon_k) - \frac{\Delta_{SDW}^2}{\omega + \varepsilon_{k-Q}} - \frac{\Delta_{SC}^2}{\omega - \varepsilon_{-k}}] \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg &= \\ -\frac{\Delta_{SDW}}{\omega + \varepsilon_{k-Q}} - [\frac{\Delta_{SDW} \Delta_{SC}}{\omega + \varepsilon_{k-Q}} + \frac{\Delta_{SDW} \Delta_{SC}}{\omega - \varepsilon_{-k}}] \ll C_{-k+Q\uparrow} C_{k-Q\downarrow} \gg &\quad (3.1.21)\end{aligned}$$

Similarly equation (3.1.17) can be written as;

$$\begin{aligned} & [(\omega - \varepsilon_{-k+Q}) - \frac{\Delta_{SDW}^2}{\omega - \varepsilon_{-k}} - \frac{\Delta_{SC}^2}{\omega + \varepsilon_{k-Q}}] \ll C_{-k+Q\uparrow} C_{k-Q\downarrow} \gg = \\ & \frac{\Delta_{SC}}{\omega + \varepsilon_{k-Q}} - [\frac{\Delta_{SDW}\Delta_{SC}}{\omega - \varepsilon_{-k}} + \frac{\Delta_{SDW}\Delta_{SC}}{\omega + \varepsilon_{k-Q}}] \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg \end{aligned} \quad (3.1.22)$$

From equations (3.1.21) and (3.1.22);

$$\begin{aligned} \frac{XYZ - \Delta_{SDW}^2 Y - \Delta_{SC}^2 Z}{YZ} \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg &= -\frac{\Delta_{SDW}}{Z} - \frac{\Delta_{SC}^2 \Delta_{SDW} Y [Y + Z]}{YZ [RYZ - \Delta_{SDW}^2 Z - \Delta_{SC}^2 Y]} \\ &+ \frac{\Delta_{SC} \Delta_{SDW} [Y + Z]^2}{YZ [RYZ - \Delta_{SDW}^2 Z - \Delta_{SC}^2 Y]} \\ &\times \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg \end{aligned} \quad (3.1.23)$$

Where  $X = (\omega + \varepsilon_k)$ ,  $Y = (\omega - \varepsilon_{-k})$ ,  $Z = (\omega + \varepsilon_{k-Q})$ ,  $R = (\omega - \varepsilon_{-k+Q})$ .

After some rearrangements we will get;

$$\begin{aligned} \frac{RYZ - \Delta_{SDW}^2 Z - \Delta_{SC}^2 Y^2 - \Delta_{SC} \Delta_{SDW} [Y + Z]^2}{YZ [RYZ - \Delta_{SDW}^2 Z - \Delta_{SC}^2 Y]} \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg &= \\ -\frac{\Delta_{SDW} [RYZ - \Delta_{SDW}^2 Z - \Delta_{SC}^2 Y] + \Delta_{SDW} \Delta_{SC}^2 (Y + Z)}{Z [RYZ - \Delta_{SDW}^2 Z - \Delta_{SC}^2 Y]} \end{aligned} \quad (3.1.24)$$

Applying the nesting condition, which is the necessary condition for the existence of SDW ordering and defined by the expression [17,28,29];

$$\varepsilon_k = -\varepsilon_{k\pm Q} \Rightarrow \varepsilon_{-k} = -\varepsilon_{-k\mp Q} \quad (3.1.25)$$

in equation (3.1.24) and using  $\varepsilon_k = \varepsilon_{-k}$ , and after some algebra we will get;

$$\ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = -\frac{\Delta_{SDW} [XY - \Delta_{SDW}^2 - \Delta_{SC}^2] + 2\Delta_{SDW} \Delta_{SC}^2}{[XY - \Delta_{SDW}^2 - \Delta_{SC}^2]^2 - [2\Delta_{SDW} \Delta_{SC}]^2} \quad (3.1.26)$$

Where the variables  $X$ ,  $Y$ ,  $Z$  and  $R$  should have the form;  $X = (\omega + \varepsilon_k) = R$  and  $Z = (\omega - \varepsilon_k) = Y$ . Thus

$$\ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = -\frac{\Delta_{SDW} [\omega^2 + \varepsilon_k^2 + \Delta_{SDW}^2 - \Delta_{SC}^2]}{[\omega^2 + \varepsilon_k^2 + (\Delta_{SDW} + \Delta_{SC})^2][\omega^2 + \varepsilon_k^2 + (\Delta_{SDW} - \Delta_{SC})^2]} \quad (3.1.27)$$

Where we have made a change  $\omega \longrightarrow i\omega$ . Which inturn can be written as

$$\ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = \frac{-\frac{1}{2}(\Delta_{SC} + \Delta_{SDW})}{\omega^2 + \varepsilon_k^2 + (\Delta_{SDW} + \Delta_{SC})^2} + \frac{\frac{1}{2}(\Delta_{SC} - \Delta_{SDW})}{\omega^2 + \varepsilon_k^2 + (\Delta_{SDW} - \Delta_{SC})^2} \quad (3.1.28)$$

$$\ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = \frac{1}{2} \sum_{\alpha=1,2} (-1)^\alpha \frac{\Delta_\alpha(k)}{\omega_n^2 + E_\alpha^2(k)} \quad (3.1.29)$$

Where;  $\Delta_\alpha(k) = \Delta_{SC} - (-1)^\alpha \Delta_{SDW}$

$$E_\alpha(K) = \sqrt{\varepsilon_k^2 + \Delta_\alpha^2(k)}$$

The order parameter of SDW is given by an expression;

$$\Delta_{SDW} = -\frac{U}{\beta} \sum_{k,n} \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg \quad (3.1.30)$$

Thus inserting equation (3.1.29) in equation (3.1.30) we will get;

$$\Delta_{SDW} = -\frac{U}{2\beta} \sum_{k,n,\alpha=1,2} (-1)^\alpha \frac{\Delta_\alpha(k)}{\omega_n^2 + E_\alpha^2(k)} \quad (3.1.31)$$

Where  $\omega_n$  is Matsubara frequency which can be given by;

$$\omega_n = (2n + 1) \frac{\pi}{\beta} \quad (3.1.32)$$

Thus equation (3.1.31) can be written as

$$\Delta_{SDW} = -\frac{U}{4} \sum_{k,\alpha=1,2} (-1)^\alpha \frac{\Delta_\alpha(k) \tanh(\frac{\beta E_\alpha(k)}{2})}{E_\alpha(k)} \quad (3.1.33)$$

Where we have used the equality;

$$\sum_n \frac{1}{(2n + 1)^2 \pi^2 + \gamma^2} = \frac{\tanh(\frac{\gamma}{2})}{2\gamma} \quad (3.1.34)$$

### 3.1.2 The order parameter of superconductivity

In the previous section we have derived the expression for SDW order parameter as a function of both order parameters and temperature,  $\Delta_{SDW} = \Delta_{SDW}(\Delta_{SDW}, \Delta_{SC}, T)$ . In this section our intention is to drive an expression for superconducting order parameter.  $\Delta_{SC}$  is given by the equation (3.1.3). The equation of motion for the pair can be obtained using Green's function in the same manner as before.

$$\omega \ll C_{k\uparrow}^+, C_{-k\downarrow}^+ \gg = \langle \{C_{k\uparrow}^+, C_{-k\downarrow}^+\} \rangle + \ll [C_{k\uparrow}^+, H], C_{-k\downarrow}^+ \gg \quad (3.1.35)$$

Where the hamiltonian  $H$  is given by equation (3.1.1). The anticommutation relation between fermion operators will reduce the above equation to;

$$\omega \ll C_{k\uparrow}^+, C_{-k\downarrow}^+ \gg = \ll [C_{k\uparrow}^+, H], C_{-k\downarrow}^+ \gg \quad (3.1.36)$$

The commutation relation in rhs of (3.1.36) will become;

$$[C_{k\uparrow}^+, H] = -\varepsilon_k C_{k\uparrow}^+ - \Delta_{SDW} C_{k-Q\downarrow}^+ - \Delta_{SC} C_{-k\downarrow} \quad (3.1.37)$$

With this, equation (3.1.36) becomes;

$$(\omega + \varepsilon_k) \ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg = -\Delta_{SDW} \ll C_{k-Q\downarrow}^+ C_{-k\downarrow}^+ \gg - \Delta_{SC} \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg \quad (3.1.38)$$

Similarly the equation of motion for the first correlation in rhs of (3.1.38) will be ;

$$(\omega + \varepsilon_{k-Q}) \ll C_{k-Q\downarrow}^+ C_{-k\downarrow}^+ \gg = -\Delta_{SDW} \ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg + \Delta_{SC} \ll C_{-k+Q\uparrow} C_{-k\downarrow}^+ \gg \quad (3.1.39)$$

Still it is necessary to calculate the equation of motion for the last correlation of equation (3.1.39), and it becomes

$$(\omega - \varepsilon_{-k+Q}) \ll C_{-k+Q\uparrow} C_{-k\downarrow}^+ \gg = \Delta_{SDW} \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg + \Delta_{SC} \ll C_{-k+Q\downarrow}^+ C_{-k\downarrow}^+ \gg \quad (3.1.40)$$

Finally the equation of motion for the second correlation in equation (3.1.38) is given by;

$$(\omega - \varepsilon_{-k}) \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg = 1 + \Delta_{SDW} \ll C_{-k+Q\uparrow} C_{-k\downarrow}^+ \gg - \Delta_{SC} \ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg \quad (3.1.41)$$

Using equations (3.1.39) and (3.1.41) equations (3.1.38) and (3.1.40) will, respectively, become;

$$\begin{aligned} & [(\omega + \varepsilon_k) - \frac{\Delta_{SDW}^2}{\omega + \varepsilon_{k-Q}} - \frac{\Delta_{SC}^2}{\omega - \varepsilon_{-k}}] \ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg = \\ & -\frac{\Delta_{SC}}{\omega - \varepsilon_{-k}} - [\frac{\Delta_{SC}\Delta_{SDW}}{\omega + \varepsilon_{k-Q}} + \frac{\Delta_{SC}\Delta_{SDW}}{\omega - \varepsilon_{-k}}] \ll C_{-k+Q\uparrow} C_{-k\downarrow}^+ \gg \end{aligned} \quad (3.1.42)$$

$$\begin{aligned} & [(\omega - \varepsilon_{-k+Q}) - \frac{\Delta_{SDW}^2}{\omega - \varepsilon_{-k}} - \frac{\Delta_{SC}^2}{\omega + \varepsilon_{k-Q}}] \ll C_{-k+Q\uparrow} C_{-k\downarrow}^+ \gg = \\ & \frac{\Delta_{SDW}}{\omega - \varepsilon_{-k}} - [\frac{\Delta_{SC}\Delta_{SDW}}{\omega - \varepsilon_{-k}} + \frac{\Delta_{SC}\Delta_{SDW}}{\omega + \varepsilon_{k-Q}}] \ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg \end{aligned} \quad (3.1.43)$$

From equations (3.1.42) and (3.1.43), after some arrangements we will get;

$$\begin{aligned} & \frac{[XYZ - Y\Delta_{SDW}^2 - Z\Delta_{SC}^2]^2 - [\Delta_{SC}\Delta_{SDW}(Y + Z)]^2}{YZ[RYZ - Z\Delta_{SDW}^2 - Y\Delta_{SC}^2]} \ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg = \\ & \frac{-\Delta_{SC}[RYZ - Z\Delta_{SDW}^2 - Y\Delta_{SC}^2] - \Delta_{SC}\Delta_{SDW}^2(Y + Z)}{Y[RYZ - Z\Delta_{SDW}^2 - Y\Delta_{SC}^2]} \end{aligned} \quad (3.1.44)$$

Applying the nesting condition and the same approximation as in the previous subsection case, equation(3.1.44) will becomes;

$$\ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg = \frac{-\Delta_{SC}[\omega^2 - \varepsilon_k^2 + \Delta_{SDW}^2 - \Delta_{SC}^2]}{[\omega^2 - \varepsilon_k^2 - \Delta_{SDW}^2 - \Delta_{SC}^2]^2 - [2\Delta_{SC}\Delta_{SDW}]^2} \quad (3.1.45)$$

which can be written as;

$$\ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg = \frac{-\frac{1}{2}(\Delta_{SC} + \Delta_{SDW})}{\omega^2 - \varepsilon_k^2 - (\Delta_{SC} + \Delta_{SDW})^2} + \frac{-\frac{1}{2}(\Delta_{SC} - \Delta_{SDW})}{\omega^2 - \varepsilon_k^2 - (\Delta_{SC} - \Delta_{SDW})^2} \quad (3.1.46)$$

After changing  $\omega \rightarrow i\omega$  and using the already defined representations  $\Delta_\alpha(k)$  and  $E_\alpha(k)$  equation(3.1.46) can have a form;

$$\ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg = \frac{1}{2} \sum_{\alpha=1,2} \frac{\Delta_\alpha(k)}{\omega^2 + E_\alpha^2(k)} \quad (3.1.47)$$

The order parameter of superconductor,  $\Delta_{SC}$ , is given by an expression;

$$\Delta_{SC} = \frac{V}{\beta} \sum_{k,n} \ll C_{k\uparrow}^+ C_{-k\downarrow}^+ \gg \quad (3.1.48)$$

$$\Delta_{SC} = \frac{V}{2\beta} \sum_{k,n,\alpha=1,2} \frac{\Delta_\alpha(k)}{\omega_n^2 + E_\alpha^2(k)} \quad (3.1.49)$$

By using the Matsubara's frequency and equation(3.1.34) equation(3.1.49) can be rewritten as;

$$\Delta_{SC} = \frac{1}{4} V \sum_{k,\alpha=1,2} \frac{\Delta_\alpha(k) \tanh(\frac{\beta E_\alpha(k)}{2})}{E_\alpha(k)} \quad (3.1.50)$$

## 3.2 Coexistence of SDW and Triplet Superconductivity

Triplet superconductivity appears provided that we have coexistence of singlet superconductivity and SDW antiferromagnetism. In many high  $T_c$  superconductors, superconducting mechanism is attributed to strong coulomb interactions of the electrons in the system, which can also be the cause for the appearance of SDW state. And this suggests that the existence of competition between the two states [30]. We review the properties of the unconventional triplet superconductivity and SDW with an emphasis on the analysis of their order parameter. Hence, in this section we want to drive an expressions for the order parameters of SDW,  $\Delta_{SDW}$ , and triplet superconductivity,  $\Delta_{SC}$ , as a function of both of them and temperature, and to compare

the variation of each with temperature. Still we can use the Hamiltonian given by equation(3.1.1), but in this case the superconducting order parameter depends on spin alignment [31] and they can be expressed as;

$$H = \sum_{p\sigma} \varepsilon_p C_{p\sigma}^+ C_{p\sigma} + \Delta_{SDW} \sum_p C_{p+Q\uparrow}^+ C_{p\downarrow} + C_{p\downarrow}^+ C_{p+Q\uparrow} + \frac{1}{2} \sum_{p\sigma} \Delta_{p\sigma}^* C_{-p\sigma} C_{p\sigma} + \Delta_{p\sigma} C_{p\sigma}^+ C_{-p\sigma}^+ \quad (3.2.1)$$

where the superconducting order parameter is given by;

$$\Delta_{k'\sigma} = \sum_k V_{k'k} \langle C_{k\sigma}^+ C_{-k\sigma}^+ \rangle \quad (3.2.2)$$

### 3.2.1 Superconducting Order Parameter

As we have done in the previous section, to drive the expression for order parameter of superconductor, we shall start from the equation of motion of the correlation that appear in equation (3.2.2);

$$\begin{aligned} \omega \ll C_{k\sigma}^+ C_{-k\sigma}^+ \gg &= \ll \{C_{k\sigma}^+, C_{-k\sigma}^+\} \gg + \ll [C_{k\sigma}^+, H], C_{-k\sigma}^+ \gg \\ &= \ll [C_{k\sigma}^+, H], C_{-k\sigma}^+ \gg \end{aligned} \quad (3.2.3)$$

Solving for commutation in RHS of equation (3.2.3) as in the previous case and using the assumption  $\delta_{\sigma,\downarrow} = 1; \delta_{\sigma,\uparrow} = 0$  we will get;

$$[C_{k\sigma}^+, H] = -\varepsilon_k C_{k\downarrow}^+ - \Delta_{SDW} C_{k+Q\uparrow}^+ + \frac{1}{2} (\Delta_{-k\downarrow} C_{-k\downarrow} - \Delta_{k\downarrow} C_{-k\downarrow}) \quad (3.2.4)$$

The nesting property of the Fermi surface that expected for low dimensional band structure and attributed to the SDW ordering gives as an expression  $\Delta_{-k} = -\Delta_k$ . Thus, using this relation, equation (3.2.4) will reduce to;

$$[C_{k\sigma}^+, H] = -\varepsilon_k C_{k\downarrow}^+ - \Delta_{SDW} C_{k+Q\uparrow}^+ - \Delta_{k\downarrow} C_{-k\downarrow} \quad (3.2.5)$$

By inserting equation (3.2.5) in equation(3.2.3) we will get;

$$(\omega + \varepsilon_k) \ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg = -\Delta_{SDW} \ll C_{k+Q\uparrow}^+ C_{-k\downarrow}^+ \gg -\Delta_{k\downarrow} \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg \quad (3.2.6)$$

In this section, we are dealing with only the triplet pair. So we ignor the singlet correlation from equation (3.2.6).

$$(\omega + \varepsilon_k) \ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg = -\Delta_{k\downarrow} \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg \quad (3.2.7)$$

The equation of motion for correlation in RHS of (3.2.7) is written as;

$$\omega \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg = 1 + \ll [C_{-k\downarrow}, H], C_{-k\downarrow}^+ \gg \quad (3.2.8)$$

$$[C_{-k\downarrow}, H] = \varepsilon_{-k} C_{-k\downarrow} + \Delta_{SDW} C_{-k+Q\uparrow} - \Delta_{k\downarrow} C_{k\downarrow}^+ \quad (3.2.9)$$

Thus using equation (3.2.9), equation (3.2.8) will become;

$$(\omega - \varepsilon_{-k}) \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg = 1 + \Delta_{SDW} \ll C_{-k+Q\uparrow} C_{-k\downarrow}^+ \gg -\Delta_{k\downarrow} \ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg \quad (3.2.10)$$

Where the correlation in RHS of (3.2.10) can be written as;

$$\omega \ll C_{-k+Q\uparrow} C_{-k\downarrow}^+ \gg = \ll [C_{-k+Q\uparrow}, H], C_{-k\downarrow}^+ \gg \quad (3.2.11)$$

Which can be rewritten, after solving the commutation relation and removing the singlet pair, as;

$$(\omega - \varepsilon_{-k+Q}) \ll C_{-k+Q\uparrow} C_{-k\downarrow}^+ \gg = \Delta_{SDW} \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg \quad (3.2.12)$$

From equations (3.2.10) and (3.2.12) we will get;

$$(\omega - \varepsilon_{-k}) \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg = 1 + \frac{\Delta_{SDW}^2}{\omega - \varepsilon_{-k+Q}} \ll C_{-k\downarrow} C_{-k\downarrow}^+ \gg -\Delta_{k\downarrow} \ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg \quad (3.2.13)$$

With the help of equation (3.2.13), equation (3.2.7) reduce to;

$$\frac{XYR - X\Delta_{SDW}^2 - R\Delta_{k\downarrow}^2}{YR - \Delta_{SDW}^2} \ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg = \frac{-\Delta_{k\downarrow} R}{YR - \Delta_{SDW}^2} \quad (3.2.14)$$

Which inturn can be written as;

$$\ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg = \frac{-\Delta_{k\downarrow} R}{XYR - X\Delta_{SDW}^2 - R\Delta_{k\downarrow}^2} \quad (3.2.15)$$

If we apply the nesting condition expressed in equation (3.1.25), equation (3.2.15) will become;

$$\ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg = \frac{-\Delta_{k\downarrow}}{XY - \Delta_{SDW}^2 - \Delta_{k\downarrow}^2} \quad (3.2.16)$$

After replacing the values of X and Y, and changing  $\omega_n \rightarrow i\omega_n$  we will get;

$$\ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg = \frac{\Delta_{k\downarrow}}{\omega_n^2 + \varepsilon_k^2 + \Delta_{SDW}^2 + \Delta_{k\downarrow}^2} \quad (3.2.17)$$

$$\ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg = \frac{\Delta_{k\downarrow}}{\omega_n^2 + E_k^2} \quad (3.2.18)$$

Where  $E_k^2 = \varepsilon_k^2 + \Delta_{SDW}^2 + \Delta_{k\downarrow}^2$ . Thus the order parameter of superconductor is given by;

$$\Delta_{k\downarrow} = \frac{V}{\beta} \sum_{k,n} \ll C_{k\downarrow}^+ C_{-k\downarrow}^+ \gg \quad (3.2.19)$$

$$\Delta_{k\downarrow} = \frac{V}{\beta} \sum_{k,n} \frac{\Delta_{k\downarrow}}{\omega_n^2 + E_k^2} \quad (3.2.20)$$

Finally by using equations (3.1.32) and (3.1.34), the order parameter is given by an expression;

$$\Delta_{k\downarrow} = V \sum_{\mathbf{k}} \frac{\Delta_{k\downarrow} \tanh\left(\frac{\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{SDW}^2 + \Delta_{k\downarrow}^2}}{2k_B T}\right)}{2\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{SDW}^2 + \Delta_{k\downarrow}^2}} \quad (3.2.21)$$

By taking an approximation over the superconducting order parameter, such that it is independent of wave vector, finally, we will come up with an expression;

$$1 = V \sum_{\mathbf{k}} \frac{\tanh\left(\frac{\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{SDW}^2 + \Delta_{\downarrow}^2}}{2k_B T}\right)}{2\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{SDW}^2 + \Delta_{\downarrow}^2}} \quad (3.2.22)$$

### 3.2.2 SDW Order Parameter

The order parameter of SDW is given by equation (3.1.2). To evaluate the term in RHS of this equation we need to calculate the equation of motion for the pair, following similar way to the previous sections.

$$\begin{aligned}\omega \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg &= \langle \{C_{k\uparrow}^+ C_{k-Q\downarrow}\} \rangle + \ll [C_{k\uparrow}^+, H], C_{k-Q\downarrow} \gg \\ &= \ll [C_{k\uparrow}^+, H], C_{k-Q\downarrow} \gg\end{aligned}\quad (3.2.23)$$

After calculating the commutation relation equation (3.2.23) can be written as;

$$(\omega + \varepsilon_k) \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = -\Delta_{SDW} \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg - \Delta_{k\uparrow} \ll C_{-k\uparrow} C_{k-Q\downarrow} \gg\quad (3.2.24)$$

By removing the singlet correlation from the above expression it will reduce to;

$$(\omega + \varepsilon_k) \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = -\Delta_{SDW} \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg\quad (3.2.25)$$

The correlation in RHS of equation (3.2.25) can be expressed as;

$$\begin{aligned}\omega \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg &= \langle \{C_{k-Q\downarrow}^+ C_{k-Q\downarrow}\} \rangle + \ll [C_{k-Q\downarrow}^+, H], C_{k-Q\downarrow} \gg \\ &= 1 + \ll [C_{k-Q\downarrow}^+, H], C_{k-Q\downarrow} \gg\end{aligned}\quad (3.2.26)$$

and after evaluating the commutation we can write it in the following form;

$$(\omega + \varepsilon_{k-Q}) \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg = 1 - \Delta_{SDW} \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg - \Delta_{k-Q\downarrow} \ll C_{-k+Q\downarrow} C_{k-Q\downarrow} \gg\quad (3.2.27)$$

The equation of motion for the last correlation in RHS of (3.2.27) is;

$$\omega \ll C_{-k+Q\downarrow} C_{k-Q\downarrow} \gg = \ll [C_{-k+Q\downarrow}, H], C_{k-Q\downarrow} \gg\quad (3.2.28)$$

which can be rewritten as;

$$(\omega - \varepsilon_{-k+Q}) \ll C_{-k+Q\downarrow} C_{k-Q\downarrow} \gg = \Delta_{SDW} \ll C_{-k+2Q\uparrow} C_{k-Q\downarrow} \gg - \Delta_{k-Q\downarrow} \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg \quad (3.2.29)$$

Neglecting the singlet pair leads us to an expression;

$$(\omega - \varepsilon_{-k+Q}) \ll C_{-k+Q\downarrow} C_{k-Q\downarrow} \gg = -\Delta_{k-Q\downarrow} \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg \quad (3.2.30)$$

From the equations (3.2.27) and (3.2.30) we will get;

$$\frac{(\omega + \varepsilon_{k-Q})(\omega - \varepsilon_{-k+Q}) - \Delta_{k-Q\downarrow}^2}{\omega - \varepsilon_{-k+Q}} \ll C_{k-Q\downarrow}^+ C_{k-Q\downarrow} \gg = 1 - \Delta_{SDW} \ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg \quad (3.2.31)$$

With the help of equation (3.2.31), equation (3.2.25) becomes;

$$\ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = \frac{-\Delta_{SDW} R}{XZR - \Delta_{k-Q\downarrow}^2 X - \Delta_{SDW}^2 R} \quad (3.2.32)$$

Applying the nesting condition, changing  $\omega_n \rightarrow i\omega_n$ , and replacing the parameters X, Z, and R by their values will reduce equation (3.2.32) to;

$$\ll C_{k\uparrow}^+ C_{k-Q\downarrow} \gg = \frac{-\Delta_{SDW}}{\omega^2 - \varepsilon_k^2 - \Delta_{k-Q\downarrow}^2 - \Delta_{SDW}^2} \quad (3.2.33)$$

Then, finally, by using equations (3.1.30), (3.1.32), and (3.1.34) in equation (3.2.33) an expression for SDW order parameter becomes;

$$1 = \frac{U}{2} \sum_k \frac{\tanh\left(\frac{\sqrt{\varepsilon^2 + \Delta_{k-Q\downarrow}^2 + \Delta_{SDW}^2}}{2k_B T}\right)}{\sqrt{\varepsilon^2 + \Delta_{k-Q\downarrow}^2 + \Delta_{SDW}^2}} \quad (3.2.34)$$

With similar approximation used in the previous section, the above expression will reduce to;

$$1 = \frac{U}{2} \sum_k \frac{\tanh\left(\frac{\sqrt{\varepsilon^2 + \Delta_{\downarrow}^2 + \Delta_{SDW}^2}}{2k_B T}\right)}{\sqrt{\varepsilon^2 + \Delta_{\downarrow}^2 + \Delta_{SDW}^2}} \quad (3.2.35)$$

# Chapter 4

## Results And Discussion

The first section of the previous chapter has made focus on the effect of SDW ordering on SS, which can be investigated by relating the order parameters of the two states (SDW and SC states). Using a model Hamiltonian consisting of spin density wave and superconducting part and applying Green's function formalism we have derived an expression which shows the relation of the two order parameters and their variation with temperature. This has been done both for singlet and triplet phases of superconductivity coexisting with spin density wave. In the absence of spin density wave, the expression for both singlet and triplet cases reduces to the well known BCS result

$$1 = \frac{V}{2} \sum_{\mathbf{k}} \frac{\tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right)}{E_{\mathbf{k}}}$$

where  $E_{\mathbf{k}} = \sqrt{\varepsilon^2 + \Delta^2}$ .

From the equations (3.1.34) and (3.1.50) we can perceive as there exist effective order parameters,  $\Delta_{i=1,2} = \Delta_{SC} - (-1)^i \Delta_{SDW}$ , which can be interpreted as, SS and SDW states can interfere either destructively or constructively. On the other hand the coexistence phase of TSC and SDW doesn't show such kind of interference. The possible origin of this difference in character between SS and TSC which are

in coexistence phase with SDW can be the competition between electrons with the same spin to condensate to either state of SS or SDW, since both states involve the pairing of up and down spin quasi-particles (electron-electron and electron-hole pairings respectively), while TSC state involve pairing of electrons with the same spin.

The coexistence of SS or TS with SDW state can be studied by solving the self-consistent equations (3.1.34), (3.1.50), (3.2.22), (3.2.35) which can be solved numerically. We have solved these integral equations with the cut-off energy,  $\hbar\omega_d = 0.8\text{mev}$ . The variation of the order parameters of those states with temperature is shown in figures (4.1) and (4.2). From these figures we can easily see that the order parameters decrease as temperature increases and they completely vanish at critical temperature. But the decreasing rate is very fast at low temperature which is slightly different from the BCS case in which the order parameter decrease slowly at low temperature and it tend to vanish suddenly at critical temperature. This difference can occur because of the additional decoupling factor, SDW, that we have considered in the model system, while in BCS theory only temperature is considered as decoupling factor.

Figure (4.1) clearly demonstrates the strong competition between the two orderings namely SDW and SS emphasizing the coexistence of SDW and SS state at low temperature. As the temperature increases first SDW state and then the SS state disappears. Similarly from figure (4.2) we can see strong competition between SDW and TSC states, but in this case the region of coexistence extends to critical temperature and the order parameters of both SDW and TSC vanish simultaneously. This means the curie temperature at which magnetic ordering disappears coincides with the critical temperature. This result is supported by an experiment

on  $ZrZn_2$  which demonstrate that both superconductivity and magnetism disappear at the same point [2]. It is also possible to have curie temperature greater than critical temperature. For example the recently discovered ferromagnetic superconductor  $RuSr_2GdCu_2O_8$  have  $T_{curie} > T_c$ . while in compounds  $ErRh_4B_4$ ,  $HoMo_6H_8$  and  $ErNi_2B_2C$ ,  $T_{curie} < T_c$  [2].

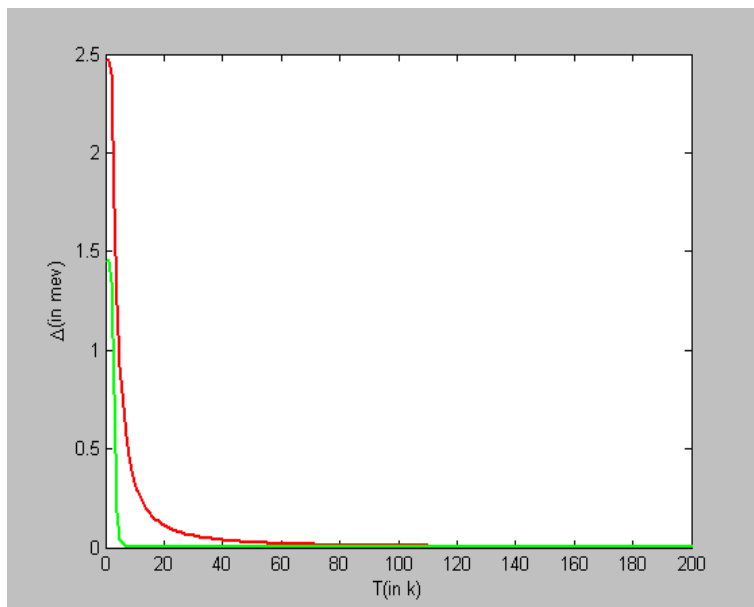


Figure 4.1: Thermal variation of SS gap and SDW gap

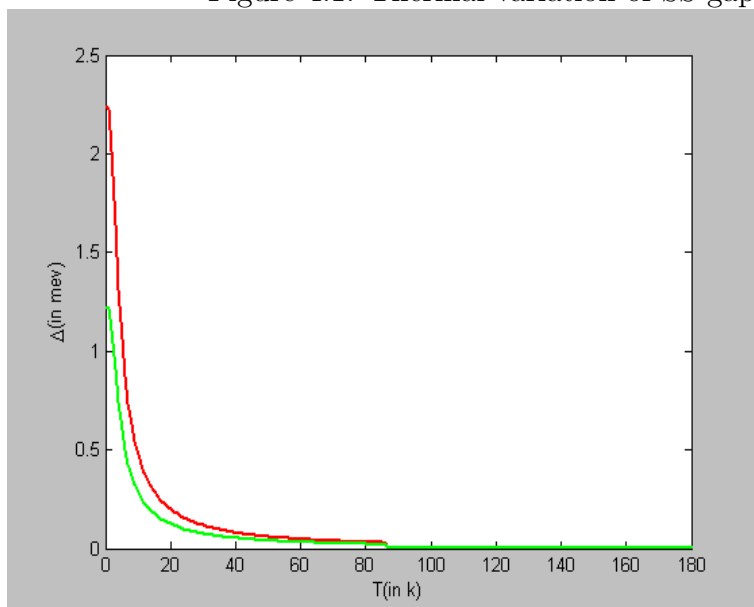


Figure 4.2: The variation of TSC gap and SDW gap with temperature

# Chapter 5

## Conclusion

In this thesis we have studied a possible coexistence of SDW and superconductivity. A model Hamiltonian of coexistence state consisting of electrons, their interaction and electron-hole interaction is studied using quantum field theory formalism of Green's function. In chapter three and four we discussed the interplay of SDW with SS and TSC where we derived expressions which demonstrate the relation between the order parameters of these states and we plot graphs which show the behavior of these order parameters with increasing temperature. It is demonstrated that there is a possibility of the two phases, spin density wave and superconductivity, coexistence region at low temperatures.

# Bibliography

- [1] K. Machida and T. Ohmi, Phys. Rev. Lett., Vol. **86**, No. 5 (2001)
- [2] S. S. Saxena et.al., Nature(London) **406**, 587 (2000); Andrew Huxley et.al., Phys. Rev. B, **63** 144519 (2001); G. Santi et.al., Phys. Rev. Lett., vol**87**, no. 24 (2001)
- [3] W. F. Brinkman, J. W. Serene, and P. W. Anderson, Phys. Rev. **A10**, 2386 (1974)
- [4] E. Dagoto, Rev. Mod. Phys. **66**, 763-840 (1994)
- [5] W. Zhang and C. A. R. Sá de Melo, arxiv:cond-mat/0502140 v1 (2005)
- [6] D. Fay and J. Appel, Phys. Rev. B **22**, 3173 (1980)
- [7] S. A. Wolf and V. Z. Krezin, Novel Superconductivity, Plenum press, New York (1987)
- [8] G. Rickayzen, Theory of superconductivity, John Wiley and sonc, Inc. (1965)
- [9] Efthimios Kaxiras, Atomic and electronic structure of solids, Cambridge University (2003)
- [10] W. Wu, Electron Correlations in Strongly Disordered Low Dimensional Systems, University of Rochester, DMR-0305428

- [11] Marko Pinterić, Electronic Properties of the Superconducting and Density Wave Phases in Organic Anisotropic Materials, Doctoral thesis, University of Zagreb(2003)
- [12] T. Ishiguro, K. Yamaji, G. Saito, Organic Superconductors, Springer-Verlag Berlin Heidelberg (1998)
- [13] James F. Annett; Superconductivity, Superfluids and Condensates, University of Bristol (2003)
- [14] M. D. Lan et. al., Chinese Journal of Physics, Vol. **38**, No. 2-II (2000)
- [15] E. Bauer and S. Bühler-Paschen, A. Prokofiev, Highly Correlated Electron Systems, Vienna University of Technology (2007)
- [16] G. Grüner, Rev. Mod. Phys., Vol.**66**, No. 1(1994)
- [17] H. Ghosh, S. Sill, S. N. Behera, arxiv:cond-mat/9903234 v1 (1999)
- [18] Overhauser A W, Phys. Rev. Lett. **4** 462 (1960)
- [19] A. M. Gabovich et. al. supercond. Sci. Technol. **14** (2001)R1-R27
- [20] G. Grüner, Rev. Mod. Phys., Vol.**60**, No. 4(1998)
- [21] C. Pasquier et.al., J. Phys. IV France **12** (2002)
- [22] I. J. Lee, Journal of the Korean Physical Society,**47**, No. 2 (2005)
- [23] Ichimura M, Fujita M and Nakao K Phys. Rev. B**43** 175(1991)
- [24] Kato M and Machida K, Phys. Rev. B **37** 1510 (1988)

- [25] Seibold G and Varlamov S, Phys. Rev. B **60** 13056 (1999)
- [26] Fawcett E, et.al., Rev. Mod. Phys. **66** 25(1994)
- [27] C. Kittel, Quantum Theory of Solid, John Wiley and Sonc. Inc. (1987)
- [28] G. C. Psaltakis and E. W. Fenton, J. Phys. C:solid state phys., **16** (1983) 3913-3932
- [29] V. P. Mineev and M. E. Zhitomirsky, Phys. Rev. B **72**, 014432 (2005)
- [30] D. F. Digor et.al., Moldavian Journal of the Physical Sciences, Vol.4, No. 4 (2005)
- [31] Y. Zhou and C. D. Gong, Europhys. Lett., **74**, No. 1, pp. 145150 (2006)

# 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.

Name: Kumneger Tadele

Signature: .....

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

Name: Prof. P. Singh

Signature: .....

Addis Ababa University

Department of Physics

July, 2007