STUDY OF COEXISTENCE OF SUPERCONDUCTIVITY AND MAGNETISM IN $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$ AND UGe_2 SUPERCONDUCTORS

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By

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DECLARATION

I here by declare that, this dissertation is my original work and has not been presented for a degree in any other university and that all sources of material used for the dissertation have been duly acknowledged.

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ABSTRACT

The coexistence of superconductivity and magnetism has recently re-emerged as a central topic in condensed matter physics due to the interplay between magnetism and superconductivity. The recent discovery of the coexistence of superconductivity(Sc) and antiferromagnetism(AFM) in high T_c superconductor(HTSc) $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$ has been studied theoretically by considering a model Hamiltonian consisting of pair interaction, intra and inter atomic Coulomb interactions, exchange interaction and scattering of Cooper pairs by magnetic moments of the gadolinium(Gd) ions. Using double time temperature dependent Green's function formalism and a suitable decoupling approximation, the coexistence of superconductivity and antiferromagnetism has been demonstrated to be a distinct possibility in $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$. The coexistence of superconductivity and ferromagnetism(Fm) in a ferromagnet UGe_2 has also been shown theoretically by considering a model Hamiltonian and employing the Green's function formalism. Furthermore, the variation of the Curie temperature(T_m) with pressure in UGe_2 has been examined and investigated. The phase diagrams of the coexistence of superconductivity and magnetism in the above mentioned superconductors have been drawn which are in broad experimental agreement.

Keywords: $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$, UGe_2, coexistence of superconductivity and magnetism, superconducting order parameter, magnetic order parameter, antiferromagnetism, ferromagnetism, Ne'el temperature, Curie temperature, phase diagram.

1. SUPERCONDUCTIVITY AND MAGNETISM

1.1 General Introduction

Superconductivity, which is the state of zero resistance was first discovered by Kamerlingh Onnes in 1911[1]. In 1908 Onnes liquified helium(He^4) by cooling it to 4.0K which consequently enabled him to cool other materials closer to absolute zero, where the energy of the materials becomes as small as possible. Onnes began to investigate the electrical properties of metals at extremely low temperatures. It had been known for many years that the resistance of metals falls when cooled below room temperature, but it was not known to what limiting value the resistance would approach if the temperature were reduced to very close to absolute zero. Some researchers believed that the electrons flowing through a conductor would come to a complete halt as the temperature approached absolute zero, others thought that a cold wire's resistance would dissipate as the temperature reduces. These ideas suggested that there would be a steady decrease in the electrical resistance allowing for better conduction of electricity. Onnes passed current through pure mercury wire and measured its resistance as he steadily lowered the temperature. He found that, the electrical resistance of pure mercury(Hg)dropped abruptly to almost zero upon cooling to below 4.2K as shown in Fig.1.0. Current was flowing through the mercury wire and nothing was stopping it.

Onnes concluded that mercury had passed into a new state, which on account of its remarkable electrical properties he called a superconductive state.

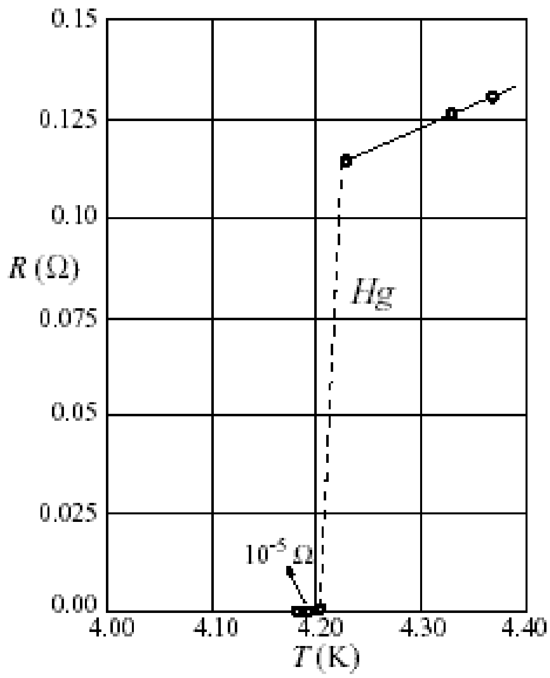

Fig. 1.1: Experimental data obtained in mercury by Kamerlingh Onnes in 1911 showing for the first time the transition from the resistive state to the superconducting state.

Onnes found that superconductors exhibit persistent current flow in a closed superconducting wire without electrical potential driving force or without damping. The temperature at which the resistance of a superconducting material vanishes is known as transition temperature(T_c). Following Onnes' discovery, many other materials including metals, alloys and complex ceramics or organic compounds such as Al(T_c=1.2K), Tl(T_c=2.4K), Sn(T_c=3.7K), La(T_c=6K), Pb(T_c=7.2K), Nb(T_c=9.2K),

La_3In(T_c=10K), Nb_3Al(T_c=17.5K), Nb_3Sn(T_c=18.4K), K_3C_{60}(T_c=19.5K), Rb_3C_{60} (T_c=30K), MgB_2(T_c=39K), etc. were found to superconduct and a record, T_c= 23K for Nb_3Ge was obtained which remained unbeaten for more than half a century. Experimental and theoretical efforts were made to understand the microscopic origin of superconductivity. In 1934 Göter and Casimir[2] introduced a phenomenological theory of superconductivity based on the assumption that in the superconducting state, there are two components of the conducting electron fluid - normal and superconducting. The properties of the normal electrons are identical to those of the electron system in a normal metal, whereas, the superconducting electrons are responsible for the anomalous properties. The super-electrons experience no scattering, have zero entropy(perfect order) and long coherence length(ξ). The two - fluid model proved a useful concept for analyzing, for instance, the thermal and acoustic properties of superconductors.

1.2 The Meissner Effect

In 1933, Meissner and Ochsenfeld[3] discovered one of the fundamental properties of superconductors- perfect diamagnetism. They found that when a superconductor is placed under a weak magnetic field and is cooled below its transition temperature(T_c), it expels the magnetic flux completely from its interior. This phenomenon is known as Meissner effect. The most spectacular demonstration of the Meissner effect is the levitation effect. That is, if a small bar magnet above T_c rests on a superconducting dish, the magnet will levitate above the superconducting dish when the temperature is lowered below T_c as indicated in fig. 1.2. Thus, Meissner found that no magnetic field is allowed inside a metal when it is in a superconducting state.

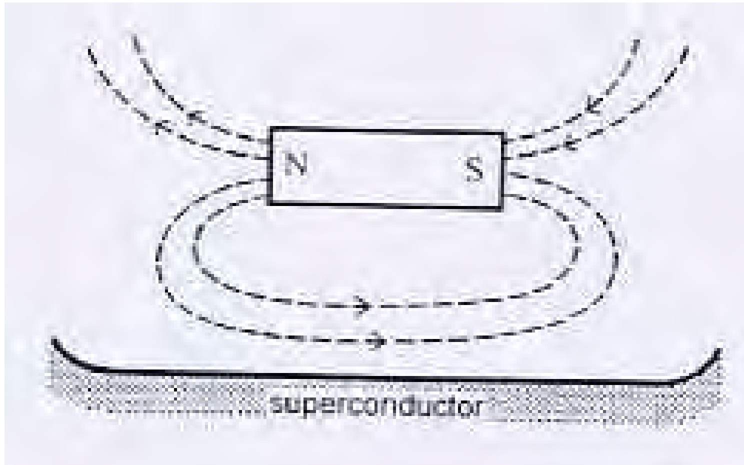

Fig. 1.2: A magnet floating in magnetic field showing Meissner effect.

Therefore, the recent discovery of compounds such as UGe_2[4], URhGe[5] and $ZrZn_2$[6] that are both magnetic and superconducting at the same time came as a big surprise to many physicists since they have long thought of magnetism and superconductivity as being mutually exclusive.

Following the discovery of the Meissner effect, in 1935 two London brothers[7], proposed a semi-phenomenological theory which dwelt basically on electron dynamic properties and the quantum phenomenon of superconductivity on a macroscopic scale. Based on this theory, they forwarded two equations to govern the microscopic(local) electric and magnetic fields. These two equations provided a description of the anomalous diamagnetism of superconductors in a weak external field. In the framework of the two-fluid model, the London equations together with the Maxwell equations describe the behavior of superconducting electrons while the normal electrons behave according to the Maxwell equations. The London equations explained not only the Meissner effect, but also provided an expression for the first characteristic length of superconductivity known as the London penetration length(λ_L).

Meissner effect can be explained quantitatively using the London equations as follows.

It is well known that, in a superconducting state the current density (J_s) is directly proportional to the vector potential field ($\mathbf{A}$) of the local magnetic field ($\mathbf{B}$).

That is,

$$\mathbf{J_s} = -\frac{\mathbf{A}}{\mu_0 \lambda_L^2} \tag{1.0}$$

where, $\nabla \times \mathbf{A} = \mathbf{B}$ and μ_0 is the permeability of free space

Taking the curl of eq.(1.0) from left, we get

$$\nabla \times \mathbf{J_s} = -\frac{\mathbf{B}}{\mu_0 \lambda_L^2} \tag{1.1}$$

From Maxwell's equations we obtain,

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J_s} \tag{1.2}$$

Taking curl of eq.(1.2) from left we get,

$$\nabla^2 \mathbf{B} = -\mu_0 \nabla \times \mathbf{J_s} \tag{1.3}$$

From eqs.(1.1) and (1.3) we obtain,

$$\nabla^2 \mathbf{B} - \frac{\mathbf{B}}{\lambda_L^2} = \mathbf{0} \tag{1.4}$$

Eq(1.4) has a solution given by

$$B(x) = B(0)\exp(-\frac{x}{\lambda_L}) \tag{1.5}$$

where

$$\lambda_L = (\frac{mc^2}{4\pi n_s e^2})^{\frac{1}{2}}$$

and is the London magnetic field penetration depth, n_s is the number density of superconducting paired electrons and $B(0)$ is the magnetic field at x=0.

Eq.(1.5) accounts for the Meissner effect and implies that the magnetic field is exponentially screened from the interior of a pure superconductor with a penetration depth of λ_L as shown in fig.1.3.

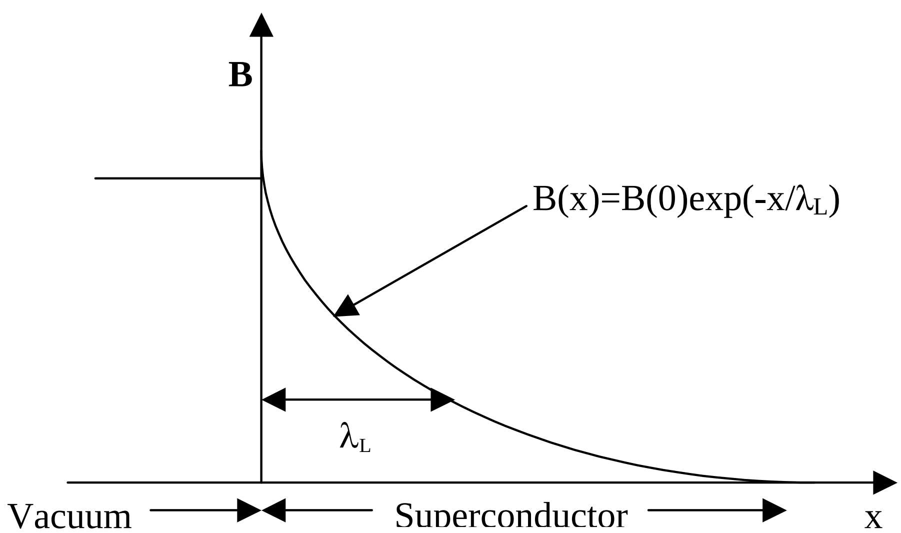

Fig. 1.3: Penetration of Magnetic Field into a Superconducting Material.

Although special attention has been paid to superconductivity, it took more than half a century to be able to reach a logical understanding.

In 1950, Fr$\ddot{o}$hlich[8] proposed that vibrating atoms of a material must play an important role causing it to superconduct. He suggested that, searching for an isotope effect in superconductors would establish whether or not lattice vibrations play some role in the interaction responsible for the onset of superconductivity. The electron-phonon interaction gives a scattering from a Bloch state defined by the wave vector $\mathbf{k}$ to $\mathbf{k}'$(where $\mathbf{k}'= \mathbf{k} \pm \mathbf{q}$ - absorption and or emission of phonons of wave vector $\mathbf{q}$). It is this interaction which is responsible for thermal scattering. Its contribution to the energy can be estimated by making a canonical transformation which eliminates the linear electron-phonon interaction terms from the Hamiltonian. Following this proposal, the isotope effect was found in 1950 independently by Maxwell[9] and Reynolds et al[10]. The study of different superconducting isotopes of mercury established a relationship between the critical temperature(T_c) and the isotope mass(M)which is given by $T_c M^{\alpha}$ = constant, where $\alpha = \frac{1}{2}$, for most superconducting materials. It is believed that the isotope effect had played a decisive role in the development of the microscopic theory of superconductivity. Ginzburg and Landau proposed an intuitive phenomenological theory of superconductivity. The theory uses the general theory of the second-order phase transition developed by Landau. The equations formulated from this theory are highly non-trivial and their validity was proven later on the basis of the microscopic theory. The Ginzburg-Landau theory played an important role in understanding the physics of the superconducting state. Furthermore, the theory is capable of describing the behavior of both conventional and unconventional superconductors in strong magnetic fields, provides an expression for the penetration length similar to the London equations and also an expression for the second characteristic length known as the Ginzburg-Landau coherence length(ε_{GL}).

1.3 The BCS Theory

Following Fröhlich's speculation, Bardeen, Cooper and Schriffer(here after denoted by BCS)[11] formulated the microscopic theory of superconductivity. The BCS theory is a microscopic field theoretical framework for treating a fermion system in which an effective attractive interaction brings about a phase coherent pair condensate with strong spatial overlap of fermion pairs. The energy of a single pair drifting relative to the condensate is discontinuously increased by the action of the Pauli principle. The basic idea of the BCS theory is that electrons(fermions) pair up via phonon coupling and the pairs(bosons) condense into a single macroscopic quantum state and travel together cooperatively and coherently through the crystal lattice without scattering. The electrons in a superconductor are ordered at and below a transition temperature(T_c) and disordered above it. It is a well known fact that, electrical resistance arises by the scattering of electrons due to defects, impurities and thermal vibrations in the crystal lattice of a conductor. However, the binding of electrons in Cooper pairs eliminates scattering and so electrical resistance disappears. Above the transition temperature(T_c), thermal vibrations disrupt the Cooper pairs and the material becomes resistive again. Furthermore, intense magnetic fields and high currents can disrupt the Cooper pairs and destroy superconductivity. The BCS theory explains how electrons form pairs known as Cooper pairs which are the building blocks of the superconducting state.

It was shown by Cooper that electrons which normally repel each other must feel an overwhelming attraction in superconductors. The pairing of electrons takes place through an intermediary lattice vibration known as phonons. According to the BCS theory, as an electron passes by a positively charged ion in the lattice of a superconductor, the electron polarizes the atom around it. This polarization of the lattice causes phonons to be emitted which form a trough of positive charges around the electron. As a result, a wave of lattice distortion due to attraction to a moving electron is created as shown in fig 1.4.

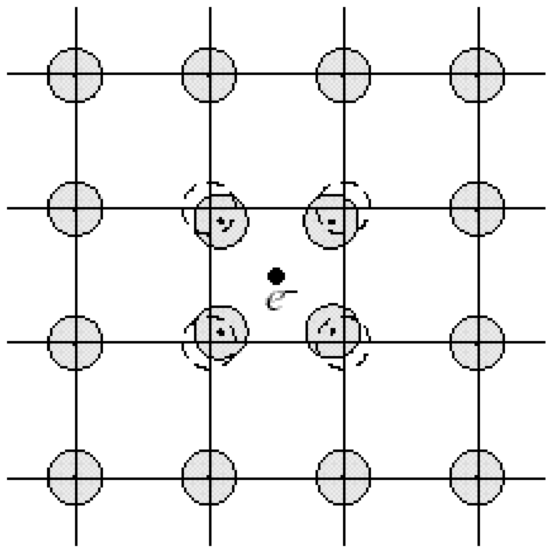

Fig. 1.4: As an electron passes between a positively charged metal ions in a lattice, the ions are attracted inward. This polarization of a lattice creates a region of enhanced positive charge which in turn attracts another electron to this region.

Before the electron passes by and before the lattice springs back to its original position, a second electron is drawn into the trough and interacts with the polarization. It is this lattice vibration that causes the two electrons(which normally repel each other) attract each other to form Cooper pairs. In this way, conventional superconductivity is mediated by the tiny lattice vibrations or phonons which accompany the motion of the electrons. The forces exerted by the phonons overcome the natural repulsion of the electrons and are screened by the phonons and are separated by a distance equal to the coherence length(ξ). When one of the electrons that makes up a Cooper pair passes close to an ion in the crystal lattice, the attraction between the negative electron and the positive ion causes vibration to pass from ion to ion until the other electron of the pair absorbs the phonon. The net effect is that an electron has emitted a phonon and another electron has absorbed the emitted phonon as shown in fig 1.5. It is this exchange of phonon that creates a Cooper Pair.

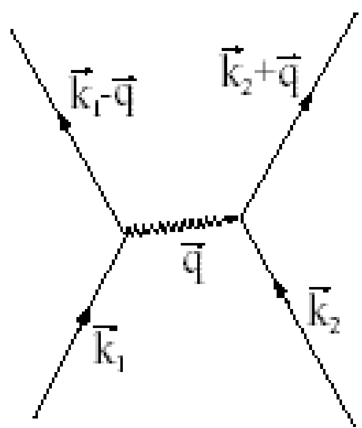

Fig. 1.5: Diagram illustrating electron-electron interaction via exchange of phonons.

The central feature of the BCS theory is that the one particle orbital are occupied in pairs. That is, if an orbital with wave vector $\mathbf{k}$ and spin up($\mathbf{k}\uparrow$) is occupied then the orbital with wave vector$-\mathbf{k}$ and spin down($-\mathbf{k}\downarrow$) is also occupied. If $\mathbf{k}\uparrow$ is vacant then $-\mathbf{k}\downarrow$ is also vacant. This leads to the formation of Cooper pairs.

The superconducting state as any state of matter has its own basic properties. So any superconductor regardless of the mechanism of supercondudctivity and the material, will exhibit the following basic properties. These are, zero resistance(infinite conductivity), a second-order phase transition at T_c, the Meissner effect ($\mathbf{B} = \mathbf{0}$), the dependence of T_c on isotopic mass(M) given by $T_c M^{\frac{1}{2}}$ = constant, the magnetic flux quantization, the Josephson effect, the presence of an energy gap in elementary excitation energy spectrum and the proximity effect. Furthermore, the BCS theory explains a gap in a superconducting phase and clears up the mystery of why the magnetic flux is quantized in units of $\frac{\hbar}{2e}$ rather than $\frac{\hbar}{e}$ confirming the pairing of electrons. Superconductivity is one of the most fascinating phenomena of modern Physics. It has had far reaching influence in many different domains of physics and has shown a tremendous capacity for cross fertilization to say nothing of its numerous technological applications. High T_c superconductors have been the darlings of materials science because they can transfer electrical current with no resistance or heat loss which have been demonstrated for some technological applications such as superconducting magnetic sensors, magnetic resonance imaging(MRI), power transmission, energy storage technology, telecommunications, computing systems, microwave filters in cellular phone based stations, etc. Superconductors are potentially some of the greatest technological triumph of the modern world if they could just be made to operate at high temperatures which would require a much better understanding of the basic principles of superconductivity at the microscopic level.

Although phonon exchange seems capable of producing transition temperature below 30K, it is more difficult to imagine that it can be responsible for high T_c superconductors($T_c \geq$ 90K) as obtained in some compounds[12]. As was stated earlier, in spite of all efforts made so far, scientists were unable to raise the transition temperature(T_c) higher than 23K for more than half a century[13].

Superconductivity in the high T_c cuprates was discovered by Bednorz and M$\ddot{u}$ller in 1986[14], when lanthanum in copper oxide(La_2CuO_4), which is an insulator is partially replaced by barium ($La_{2-x}Ba_xCuO_4$), becomes a superconductor with a transition temperature of about 36K. The discovery of this new material remains a challenge to theorists and there is still no unambiguous theoretical explanation for this phenomenon. It is well known that depending on the temperature and on the level of doping, cuprates can be insulators, normal metals or superconductors. At low temperatures and in the absence of doping, the parent compound is an antiferromagnetic Mott insulator. As the number of carriers is increased, the system becomes superconducting until for very large value of dopant(x) metallic behavior is observed down to the lowest temperatures. The superconducting critical temperature$T_c(x)$ traces a dome as shown in fig.1.6. Samples with the maximum T_c are called optimally doped while samples on either side of the optimally doped regime are called underdoped or overdoped regimes respectively.

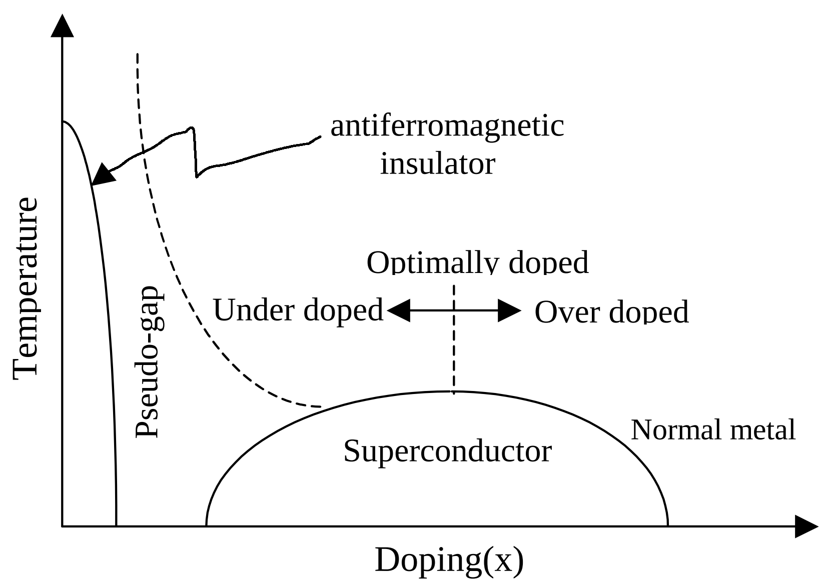

Fig. 1.6: Schematic phase diagram of high T_c superconductors with doping.

It was a surprise to observe superconducting in copper oxide based systems because no previous oxide superconductors had ever been found in their stoichiometric form. Such oxides are generally believed to be insulators. This opened flood gates to search for materials having higher transition temperatures. Within few years, a number of high T_c compounds or materials were discovered. Efforts are still on going for the search of superconductors at room temperature. Experimental investigations of high T_c cuprates reveal that cuprate families generally have parent members which are antiferromagnetic insulators such as La_2CuO_4(T_c=36K), $YBa_2Cu_3O_6$(T_c=120K), $Bi_2CaSr_2LaO_8$(T_c=110K) and $GdBa_2Cu_3O_{7-\delta}$(T_c=93K). They show highly unusual properties both in the normal and the superconducting states. High T_c superconductors exhibit the main superconducting properties that are exhibited by the conventional superconductors.

A "pseudogap" region above T_c was observed for the first time in 1989 in nuclear magnetic resonance(NMR) measurements[15]. The "pseudogap" is a partial energy gap, a depletion of the density of states above the critical temperature. For underdoped regime of cuprate ceramics, pseudogap is observed in a temperature range considerably above a superconducting transition temperature[16], which displays a partial gapping of the Fermi surface and evidence of superconducting pairing fluctuations, but no more long-range superconducting order. In the different types of copper oxides, T_c varies with electron or hole concentration, typically around 0.15-0.2 holes per CuO_2. Also, d-wave symmetry in the energy of electrons in different directions in insulating and superconducting ceramics suggest that electron pairs are formed earlier to T_c and perhaps briefly paired up and then separate again[17]. The new high T_c superconductors that were discovered are based on doped materials that are antiferromagnetic in their undoped state. Actually, before these materials were found to be superconductors, they were considered to be the best example of two dimensional quantum Heisenberg magnets.

It is believed that, the origin of superconductivity in cuprates lies in the copper oxide planes which are also the origin of the magnetism at low doping levels. Upon doping, the Ne'el temperature(T_N) decreases up to some doping level at which an ordered antiferromagnetic state cannot be found any more. Above some doping level superconductivity emerges. As is schematically illustrated in fig.1.6, the critical temperature increases with doping up to the "optimal doping" point, and increasing the doping further results in reduction of T_c.

It has been realized that, the BCS theory based on electron-phonon interaction is not perhaps capable of explaining high T_c cuprate superconductors and other materials. Hence, a number of theories have been proposed by several researchers which invoke phonons, excitons, biexcitons, plasmons, charge and spin fluctuations(magnons, spin polarons, spin bags) as mediators causing the attractive interaction between a pair of electrons [18] to explain high T_c superconductors and other unusual properties of these systems. So far, there is no general consensus on the mechanism of superconductivity in high T_c cuprate superconductors such as $RuSr_2GdCu_2O_8$, $GdBa_2Cu_3O_{7-\delta}$, $YBa_2Cu_3O_{7-\delta}$ and ferromagnetic superconductors like $ErRh_4B_4$, $HoMo_6S_8$, $ErNi_2C_2B_2$, UGe_2 and URhGe. It was found that all the high T_c cuprate superconductors are antiferromagnetic insulators in their normal state and upon doping or change of oxygen contents, antiferromagnetism seems to be destroyed making way to superconductivity. It is therefore, very natural to think that the two phenomena - superconductivity and magnetism may possibly be related more intimately.

1.4 Types Of Superconductors

Superconductors are categorized as type I(soft) and type II(hard) superconductors. The basic difference between type I and type II superconductors is simplified by their response to applied magnetic field. Type I superconductors repel completely a weak magnetic field($H < H_c$) from their interior-Meissner effect. This Type of superconductors super-conduct for fields less than the critical field H_c and above this critical value superconductivity is completely destroyed and returns to the normal state. On the other hand, type II superconductors can conduct with out resistance in a relatively large magnetic field. Compound superconductors exhibit type II magnetic behavior and tend to have higher critical fields than type I or elemental superconductors. In this case there are two important field scales, a lower critical field H_{c1} below which the material behaves like a type I superconductor, that is, in the superconducting Meissner state and an upper critical field H_{c2} above which the sample is a normal conductor. For fields between H_{c1} and $H_{c2}(H_{c1} < H < H_{c2})$ magnetic lines known as vortices penetrate the sample to produce a mixed state which super-conducts as shown in fig. 1.7. In the mixed or vortex state the normal material takes the form of threads running parallel to a field surrounded by current loops. At H_{c1} the vortices are few and far apart while at H_{c2} they overlap to such an extent that the whole sample becomes normal. The theory of type II superconductors was forwarded by Ginzburg, Landau, Abrikosov and Gorkov.

In type II superconductors, H_{c2} can be expressed in terms of H_c as,

$$H_{c2} = \frac{H_c^2}{H_{c1}} \tag{1.6}$$

where $H_c = H_0[1 - (\frac{T}{T_0})^2]$

The other main difference between type I and Type II superconductors is in

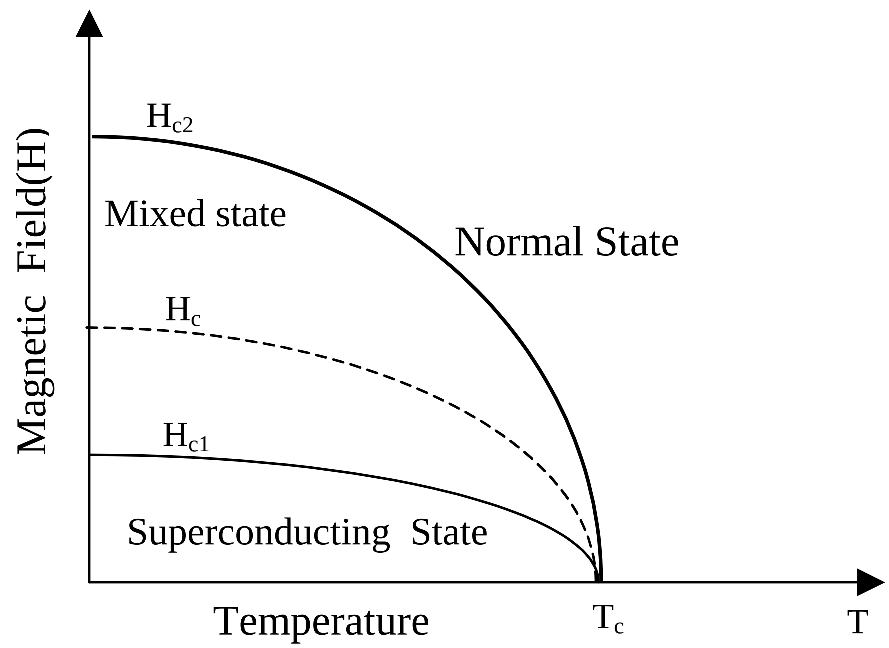

Fig. 1.7: Schematic Phase Diagram of Magnetic Field Versus Temperature.

the mean free path(ℓ_f) of the conduction electrons in the normal state. If the coherence length(ξ_{GL}) is greater than the Ginzburg-Landau magnetic field penetration depth(λ_{eff}), the superconductor will be type I and if the coherence length is shorter(since $\xi_{GL} \sim \ell_f$) than the penetration depth, the superconductor will be type II.

The critical fields H_{c1} and H_{c2} are related to each other as follows,

$$H_{c1} = \frac{H_c}{\kappa} \tag{1.7}$$

and

$$H_{c2} = \kappa H_c \tag{1.8}$$

where $\kappa = \frac{\lambda_{eff}}{\xi_{GL}}$ and is called the Ginzburg-Landau characteristic parameter.

The Ginzburg-Landau parameter is temperature independent and it phenomenologically characterizes a given superconductor. The actual criterion which determines whether a superconductor is type I or Type II is related to whether $\kappa < \sqrt{\frac{1}{2}}$ or $\kappa > \sqrt{\frac{1}{2}}$ respectively.

As was mentioned earlier, superconductivity and magnetism usually try to avoid each other. That is, superconductivity expels residual internal magnetic fields while sufficiently high magnetic field can destroy superconductivity completely. Thus, the recent discovery of compounds that are both magnetic and superconducting at the same time came as a remarkable development. As superconductivity and magnetism are to a great extent antagonistic to each other, their coexistence in homogeneous materials requires some special very reliable conditions to be fulfilled. The study of superconductivity and magnetism and their mutual coexistence or interaction has been a very important problem for the understanding of the physics of the two phenomenon for explaining a number of experimental and theoretical results, as well as for possible engineering applications. The important classes of materials or compounds showing the coexistence of superconductivity and magnetism are ternary rare earth compounds[18], $GdBa_2Cu_3O_{7-\delta}$ and uranium based compounds. Hence, the recent discovery of superconductivity near a ferromagnetic quantum critical point in UGe_2[4], $URhGe$[5] and $ZrZn_2$[6] has led to a lot of research activities to understand the possible coexistence of superconductivity and magnetism. In this study, the possible coexistence of superconductivity and magnetism in $GdBa_2Cu_3O_{7-\delta}$ and UGe_2 is theoretically investigated.

The lay out of our research work is presented as follows. In chapter 2, the review of works carried out by several workers through the years which are closely related to our research work is presented. In our work, the double time temperature dependent

Green's function formalism is used to study model Hamiltonian systems. A brief description of this mathematical technique is given in chapter 3. The theoretical formulation of the problem is presented in chapter 4. This chapter is subdivided into two sections. In section 4.1, the coexistence of superconductivity and antiferromagnetism in $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$ is studied. The model Hamiltonian is described and equations of motion have been obtained by using the Green's function formalism. These equations are solved in order to obtain various correlation functions.

In section 4.4, the coexistence of superconductivity and ferromagnetism in UGe_2 is analyzed theoretically by considering a model Hamiltonian by employing the Green's function formalism. Furthermore, the variation of the Curie temperature(T_m) with pressure is discussed in this section. Phase diagrams, have been obtained and discussed. Finally, we have summarized our findings in chapter 5.

2. REVIEW OF LITERATURE

2.1 Introduction

The search for ever increasing high T_c superconductors and mechanisms of superconductivity is one of the most challenging tasks of condensed-matter physicists and material scientists. To obtain a superconducting state reaching beyond the technological and psychological temperature barrier of 77K(the boiling point of liquid-nitrogen) will be one of the greatest triumph of scientific endeavor of this kind.

Superconductivity occurs in many metallic elements of the periodic table and their alloys, intermetallic compounds and doped superconductors. The superconducting properties of the so called low T_c superconductors are well understood in terms of the BCS theory. The discovery of high T_c superconductivity by Bednorz and M*ü*ller[14] in La-Ba-Cu-O systems has led to intensive searches for new mechanisms of superconductivity. The research on the area has been developed explosively and much attention has been given on perovskite type materials. Anderson[19], pointed out the possibility of superconductivity in strongly correlated electron systems near the metal-non-metal transition. Since then a number of theoretical studies have been made on Hubbard-type of models. All these models are based essentially on a single Cu(d) or O(p) band, although some models stress the $d_{x^2-y^2}$ character[19], while others the oxygen p character for extra holes. There are a number of theories related to high T_c superconductors that have been put forward to understand the pairing mechanisms in high T_c superconductors. The discovery of superconductivity in La(Ba,Sr)CuO(T_c =36K)[14], Y-Ba-Cu-O (T_c =90K)[20], Bi-Sr-Ca-Cu-O (T_c =110K)[21], Tl-Ca-Ba-Cu-O(T_c =120K)[22], Hg-Ba-Ca-Cu-O (T_c =164K under high applied pressure) etc. has been followed by intensive theories and experimental studies of this class of compounds and most of the researchers believe that the BCS or conventional theory is not adequate to explain the superconductivity of materials with such high transition temperatures. Fig 2.1 shows the superconducting critical temperature(T_c) of several cuprates and metallic superconductors as a function of the year of discovery.

Many new ideas and proposals have been generated for possible new mechanisms. Up to now, there are no general agreements or consensus on a single mechanism proposed to explain the origin of pairing of high T_c superconductors. The proposals regarding the pairing mechanisms that lead to high-T_c superconductors range from conventional models(pairing mediated by bosonic excitations)to exotic models based on quasi-particles in two dimensions that assume pairing through non-phononic excitations. Currently, emphasis is given to researches on copper-oxide(cuprate) superconductors some of which exhibit superconductivity at a temperature as high as 160K. These remarkable superconducting materials are of immense interest because of their potential applications in technology and the possibility that a new superconducting electron pairing mechanism different from the conventional electron-phonon interaction is responsible for their spectacularly high superconducting transition temperature.

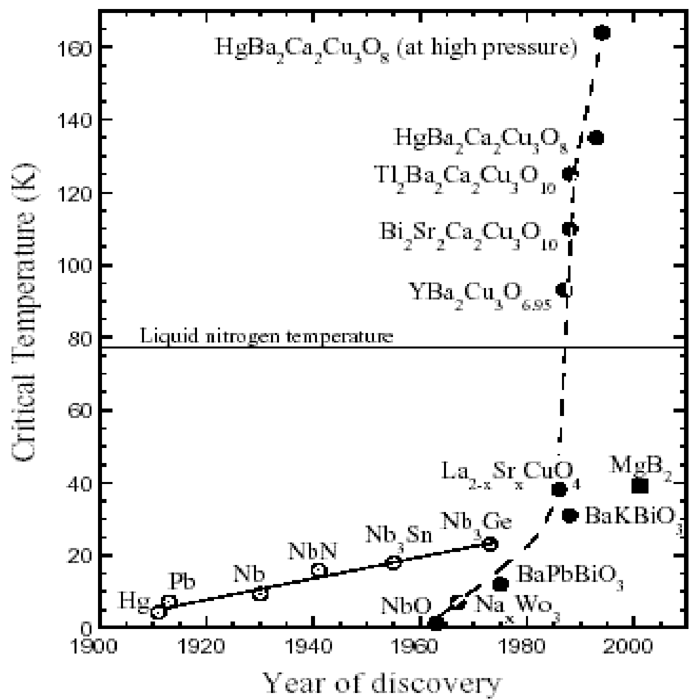

Fig. 2.1: The time evolution of the superconducting critical temperature since the discovery of superconductivity in 1911. The solid line shows the T_c evolution of metallic superconductors and the dashed line marks the T_c evolution of superconducting oxides.

In this chapter, we review the theoretical and experimental works which have been done so far by other researchers which are closely related to our work regarding pairing mechanisms and the coexistence of superconductivity and magnetism in $GdBa_2Cu_3O_{7-\delta}$, UGe_2 and related materials.

2.2 Pairing Mechanism In HTSc And Uranium Based Compounds

2.2.1 Pairing Mechanisms In High T_c Superconductors

Electrons need help to form superconducting pairs. In conventional superconductors, lattice vibrations or phonons push the electrons together into the superconducting state. The superconducting state of high T_c cuprates is basically BCS like formed by the condensation of charge 2e Cooper pairs. The first remarkable microscopic theory of superconductivity based on pairing of conduction electrons through electron lattice interaction of phonons was formulated by Bardeen, Cooper and Schrifer(BCS)[11]. They derived expressions for T_c and for the superconducting energy gap parameter(Δ) and explained experimental results of conventional superconductors. In unconventional superconductors and those with a high superconducting transition temperature(T_c), magnetic fluctuations are believed to play the role of mediating pairing. Magnetic fluctuations are strongest when magnetic order is about to form or to disappear, a point known as the quantum critical point. Here, electron spins are wobbliest and the spin fluctuations have the lowest frequencies[23].

Cohen et al[24], suggested that using phonon mechanisms, T_c cannot be raised indefinitely. In the BCS expression, T_c depends linearly on the characteristic phonon frequency known as the Debye frequency. On increasing the Debye frequency, attractive pairing interaction decreases as it varies inversely to the square of the phonon frequency(ω_D). To explain high T_c, large electron-phonon coupling is required as a result the electron would become so heavy that they would become almost immobile.

Leary et al[25], have found a small increase in T_c (from 0.3K to 0.5K) by the substitution of ^{18}O (90%) in place of ^{16}O in YBa_2CuO_7. This finding suggests that, phonons play an important role in electron pairing mechanism in YBa_2CuO_7. Batlogg et al[26], found that T_c in superconductors such as $YBa_2Cu_3O_7$ do not change significantly by replacing 75% of ^{16}O by ^{18}O. This clearly shows that weak electron-phonon coupling alone is not responsible for superconductivity in these materials. Jaejun et al [27], suggested that the nesting of the Fermi surface in $LaCuO_4$ is destroyed on doping by divalent atoms such as barium and strontium, which also suppress the structural instability and a system close to such an instability will have phonon modes of very low frequency that according to them will generate the strong pairing interaction needed to explain high critical temperature. Weber[28], suggested that phonons alone are not strong enough to explain the high T_c values in superconductors. Experimental work by Bourne et al[29], suggested that the absence of oxygen isotope shift in high T_c superconductors $YBa_2Cu_3O_{7-\delta}$ through the substitution of ^{16}O by ^{18}O shows that a non-phonon mechanism may be important in this material. As electronic and magnetic excitations are at energies higher than the phonons, they can lead to higher T_c and are considered as an alternative mechanism for pairing. Ginzburg and Little [30], independently proposed superconductivity by electronic polarization. Their proposal relied on one dimensional or on sandwich geometries in order to confine the excitations in a physically different region than the carriers. Later, Allender et al[31], put forward a new mechanism for superconductivity based on electronic theory and argued that T_c can rise up to 800K by the proposed mechanism which was later questioned by Anderson and Irikson. Alexandrov et al[32], have proposed a pairing mechanism which involves high - energy excitation such as bipolarons. Chakravarty et al[33], considered biexcitons as a possible pairing mechanisms for high T_c superconductors. Kresin [34], showed that pairing interaction in oxides is mediated not only by low frequency phonons but also by plasmons. One promising approach for high T_c pairing is based on the idea of a doped resonant valence bond(RVB)state. This mechanism was first proposed by Anderson[19] to describe a lattice of antiferromagnetically coupled spins where the quantum fluctuations are so strong that long-range magnetic ordering is suppressed. The system resonates between states in which different pairs of spins form singlet states that have zero spin and hence no fixed direction in place. The RVB state is just one of many theoretical mechanisms or approaches of pairing in high T_c superconductivity. Other competing theories include those based on fluctuating stripes and those that propose to unite the superconducting and antiferromagntic phases in a large symmetry group (so called SO(5) theories). In the superconducting cuprates such as $GdBa_2Cu_3O_{7-\delta}$, stripes are quoter filled(that is, one hole per two Cu sites)and run along -O-Cu-O-Cu- bonds[35]. The charge stripes are dynamic - they can meander and move in the transverse direction. Intrinsically, the charge stripes are insulating, that is, there is a charge gap on the stripes. However, the presence of soliton-like excitations on the stripes make them conducting. These soliton-like excitations are one dimensional polarons called polaronic solitons. They propagate in the middle of the charge gap. On cooling, the polaronic solitons give rise to pairs coupled in a singlet state due to local deformation of the lattice. Thus, the moderately strong, non-linear electron-phonon interaction is responsible for electron pairing in the cuprates. Other theories are based on the polaron mechanism and seek to exploit the strong coupling between electrons and phonons in oxide materials. Verma et al[36], suggested a purely electronic pairing mechanism for superconductivity which is specific to the electronic structure of the new oxide superconductors. They argued that, the newly discovered high T_c oxide metals have a low enough electron density that the charge transfer excitations between the

nearest neighbor cations and anions are unscreened. It was further suggested that, the high T_c is due to the scattering of electrons from such resonance rather than phonons. Alexandrov[37], has used polarons as the pairing mechanisms to explain the peculiar properties of high T_c superconductors. Sinha and Singh[38], considered super-exchange via oxygen as a possible mechanism for pairing. Furthermore, Singh and Sinha [39], have proposed a new mechanism for high T_c superconductors involving biexcitons. These biexcitons result from the possible electronic polarization of a superconducting medium in which two layers are embedded correlated charge transfer from complex $O - Cu^{+}$ - O^{-} to complex O^{2-} - Cu^{3+} - O^{2-}. It is argued that, this process may take precedence over the correlated charge transfer pair only when energies are nearly degenerate. They have proposed the possibility of explaining all possible high values of T_c. Sinha[40], has proposed a combined mechanism for an alkali doped C_{60} superconductors given by A_xC_{60}(where x=3, A= K, Rb, Cs, etc.). It consists of phononic and high energy excitation mechanisms. The latter results from the bond polarization. It involves Z-bond polarization interaction with conduction electrons and accounts for the higher T_c observed in these systems.
Pandey et al[41], have studied the role of combined mechanisms which consists of phonon and biexciton pairing mechanisms. Zho et al[42], carried out magnetization and thermal expansion measurements on copper-oxide superconductor samples and showed that polaronic charge carriers exist and condense into Cooper pairs in the copper-oxide superconductors. The presence of antiferromagnetism correlations is a very exciting feature which may play an important role in high T_c superconductivity.

Applying perturbation method, Anderson[43], derived magnetic exchange interactions in terms of V/U(V being transfer integral or hybridization matrices and U the on site repulsion). Later, these magnetic interactions were used for pairing

of electrons. It has been suggested by Emery[44], that the antiferromagnetic background of copper oxide compounds may give rise to a mechanism of strong coupling to local spin configurations which is capable of predicting high magnitude of $T_{\mathbf{C}}$. Employing Emery's model, Hirsch[45], showed that antiferromagnetic ordering of the copper moments will lead to either localization or pairing of the oxygen holes and the magnetic anisotropy is suggested to strongly enhance superconductivity in these systems. Chen et al [46], explained high temperature superconductivity in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_7$ by employing magnon-pairing mechanism. The ferromagnetic coupling of the conduction electrons with Cu(d)spins induce the attractive interaction responsible for the superconductivity leading to triplet coupled pairing. This leads to a maximum transition temperature T_c of about 200K.
Mathur et al[47], found experimental evidence that magnetic interactions can lead to high value of transition temperature under certain conditions. Experiments made by Mook et al[48], reveal that low frequency magnetic excitations are virtually identical to those of similarly doped $La_{2-x}Sr_xCuO_4$. If magnetic excitation is the pairing mechanism, it is universal in all copper-oxide systems. Ghosh et al[49], presented a model study for the coexistence of spin density wave (SDW) and superconductivity. They assumed that superconductivity is due to generalized attractive potential with a separable form without specifying to any particular origin and found d-wave symmetry of superconducting phase. Furthermore, a number of pairing mechanisms in real space pairing of electrons followed by Bose-Einstein condensation had been suggested by Schaforth[50], Noziers and Schmitt-Rink[51], which provided an alternative to Cooper pairing mechanism.

Recently, Tranquada et al[52], showed that both antiferromagnetic correlations and mobile holes can be accommodated in the same domain through charge segregation as found in recently discovered stripe phase by Zaanen [53]. In copper oxide parent compounds of the high-T_c superconductors, the valence electrons are localized-one per copper site-by strong intra-atomic Coulomb repulsion. A symptom of this localization is antiferromagnetism, where the spins of localized electrons alternate between up and down. Superconductivity appears when mobile holes are doped into this insulating state and it coexists with antiferromagnetic fluctuations[54]. After the discovery of high T_c superconductors the prime objectives of condensed matter physicists and material science researchers have been to raise the transition temperature to make materials technologically useful.

2.3 Coexistence Of Superconductivity And Magnetism

Superconductivity and magnetism seem to be similar in their appearance in the nature of their occurrence and from many other points of view. Superconductivity and magnetism tend to suppress one another. However, the existence of long - range ordering of both kinds in the same material has been established in the ternary rare earth and actinide compounds[17]. The problem of coexistence of superconductivity and magnetism has been revived following the discovery of superconductivity in the ternary rare earth(R) compounds of the RMo_6X_8 - type(where X= S, Se)[55] and RRh_4B_4 - type[56]. The renewed interest in the subject has indeed increased with the discovery of re-entrant superconductivity in $ErRh_4B_4$ and $HoMo_6S_8$. Magnetism and superconductivity are manifestations of two different ordered states into which metals can condense at low temperature and in general these states are inimical to one another. The first theoretical study on the coexistence of superconductivity and magnetic ordering was published in 1957 by Ginzburg[57].

According to Ginzburg, the coexistence of magnetism and superconductivity is almost impossible except when the ferromagntic field is smaller than the thermodynamic critical field(H_{c2}) of the superconductor. Later, Baltensperger et al[58], demonstrated that the time reversal symmetry is broken by the antiferromagnetic ordering and superconductivity may coexist with antiferromagnetism in a form of slightly modified pairing system. Neutron scattering experiments have confirmed that superconductivity and antiferromagnetism can coexist peacefully because on the average the magnetic moments in these compounds have almost no effect on the Cooper pairs as the exchange interaction is zero[59]. When the periodicity of the antiferromagnetic ordering is short compared to either the London penetration depth (λ_L) or the coherence length(ξ) of the superconductor, antiferromagnetism coexists with superconductivity since the spin fluctuations are averaged out and are ineffective in destroying the superconducting state. The first experimental investigation on the coexistence of magnetism and superconductivity was initiated by Matthias et al[60] in 1959. Abrikosov et al[61], showed that there is a critical transition paramagnetic impurity which could destroy superconductivity. They explained the suppression of T_c by magnetic impurities by treating the doped magnetic impurities in superconductors as uncorrelated. Below the critical concentration both superconductivity and magnetism can survive. On the experimental side, the magnetic impurities were introduced into the superconducting system and their effect on the suppression of superconducting transition temperature was investigated by Maple et al[17]. The presence of magnetic impurities lead to the pair-breaking effect. In a singlet superconductor, the pair breaks into two separate electrons with "up" or "down" spin which no longer belong to the condensate. This pair breaking results in the reduction of the superconducting transition temperature(T_c) and the superconducting order paramete(Δ). Gorkov et al[62], predicted the possibility of coexistence of superconductivity and magnetism in a narrow temperature range. In 1977, Matthias, Maple and Fisher discovered the possible coexistence of superconductivity and magnetic ordering in the ternary rare-earth compounds. Until the discovery of the rare-earth ternary compounds such as $ErRh_4B_4$ by Fertig et al[63] and $HoMo_6S_8$ by Ishikawa[64], it was suggested that the relation between magnetism and superconductivity was of spin glass type. The coexistence of superconductivity and magnetism in ternary rare earth compounds, such as $ErRh_4B_4$ and $HoMo_6S_8$ has been demonstrated experimentally by Fisher et al[65]. Sinha and Singh[66] studied the effect of magnetic ordering on superconductivity in some rare earth compounds and found a re-entrant behavior of the superconducting order parameter(Δ). They found that superconductivity can be destroyed at two temperatures, at T_{c1} due to thermal pair breaking and at $T_{c2}(< T_{c1})$ when $\Delta = \eta($ η being the magnetic order parameter of rare earth ions) and spin polarization of conduction electrons. Furthermore, the coexistence of superconductivity and antiferromagnetic ordering of a localized spin system has been proved in a large class of the rare earth ternary alloys. Blount et al[67], suggested that electromagnetic interactions are responsible for the sinusoidally modulated magnetic state in $HoMo_6S_8$ and $ErRh_4B_4$. Privorotsky[68], considered the influence of the spin waves on the electron-electron interaction and showed that this interaction becomes attractive only for the pairs in the triplet state with zero total spin projection, the attraction being maximum for the electrons in the p-state. Baltensperger et al[58], reconsidered this problem by taking the electron-phonon contribution in the calculation of the effective electron-electron interaction. In this way, they showed that singlet pairing is possible for the electronic time-reversed states, with a slight change in the electron-electron interaction which is weakened by the antiferromagnetic order. Bak [69], pointed out that rare earth ions in superconducting ternary compounds together with dipolar magnetic ordering should exhibit ordering of their permanent and localized quadruple moments. Fenton[70], studied the effect of static antiferromagnetic ordering on superconductivity. He explained that the only effect of static antiferromagnetism on T_c and Δ is replaced in the gap equation of the electron density of states for non-magnetic crystal by that of the antiferromagnet. The relationship between superconductivity and long-range antiferromagnetic ordering was also studied in RMo_6Se_8(R= Gd, Tb and Er) by McCallum et al [71], RRh_4B_4(R= Nd, Sm and Tm) by Hamaker et al [72], and RMo_6S_8(R= Gd, Tb, Dy and Er) by Ishikawa et al [64]. Cava et al[73], discovered a number of borocarbides of general formula RNi_2B_2C(R= Y, Tm, Ho, Dy), Grigereit et al[74], performed neutron scattering measurements on the re-entrant antiferromagnetic superconductor, $HoNi_2B_2C$ which becomes superconducting at 7.5K, re-enters the normal conducting state at 5K and quickly recovers superconductivity at lower temperature. The experiment reveals that the magnetic ordering which first forms upon cooling is oscillatory in nature and is directly coupled to superconducting order parameter. Sinha and Singh[75], considered the scattering of Cooper pairs by localized electrons along with their exchange interaction and intra and inter site interactions and obtained that the possibility of antiferromagnetic ordering in the superconducting state. The study of the interplay between magnetism and superconductivity has recently been revitalized by the discovery[76,77] of a class of compounds with the formula RNi_2B_2C which are both antiferromagnetic and superconducting at sufficiently low temperature[78]. It has been suggested[79] that magnetic ordering can coexist in these materials on an atomic scale.

Furthermore, the coexistence of superconductivity and magnetism was discovered in many compounds such as $ErNi_2B_2C$[80], $RuSr_2R_{2-x}CexCu_2O_{10}$(R= Eu and Gd, Ru-1222)[81, 82] and in $RuSr_2GdCu_2O_8$(Ru-1212)[64]. In heavy rare-earth samples(Ho, Er, Tm, Y)coexistence of superconductivity and antiferromagnetism is observed. The coexistence of superconductivity and antiferromagnetism was first discovered in $TbMo_6S_8$, $DyMO_6S_8$ and $ErMo_6S_8$[83] and subsequently in many other ternary compounds such as RMo_6S_8[84] and RRh_4B_4[85]. Hence, this type of coexistence is now believed to be rather a common phenomenon in magnetic superconductors confirming the theoretical predictions[51].

There are two sources of magnetism in metals. These are localized magnetic moments and the 'sea' of conduction electrons. Local magnetism occurs in rare earth metals due to the incomplete filling of electrons in the inner atomic shells. This leads to a well defined magnetic moment at every fixed atomic site which in turn produces long-range magnetic coupling due to the exchange of conduction electrons. The second type of magnetism - known as band magnetism arises from the magnetic moments of the conduction electrons themselves. In a metal the electrons are itinerant, that is, they are free to move from one atomic site to another atomic site and they tend to align their magnetic moments in the direction of an applied field. This also occurs in the uranium - germanium based compounds UGe_2[4], $URhGe$[5] and also in $ZrZn_2$[6], the recently discovered ferromagnetic compounds. The discovery of superconductivity at high pressure in the ferromagnetic materials such as UGe_2 raised the possibility that bulk superconductivity might be found in other ferromagnets also. Superconductivity depends crucially on the details of both the magnetic structure and the electron bands. Another important class of compounds which exhibit the interplay between superconductivity and magnetism are heavy fermion superconductors such as $CeCu_2Si_2$[86], UBe_{13}[87], UPt_3[88], URu_2Si_2, UNi_2Al_3 and UPd_2Al_3[89]. These compounds appear to exhibit an unconventional type of anisotropic superconductivity in which the superconducting electron pair is mediated by magnetic spin fluctuations and the superconducting energy gap vanishes at points or lines on the Fermi surface. After the discovery of high T_c cuprates it was found that there is a close relationship between magnetic ordering and superconductivity as these are superconductors containing magnetic Cu $3d^9$ ions, which are antiferromagnetically aligned. Tranqua et al[52], confirmed the existence of long range 3D antiferromagnetic ordering of Cu spins by using neutron diffraction experiments(NDE) on ceramic powder of $YBa_2Cu_3O_{6+\delta}$. Tang [90], had studied the coexistence of antiferromagnetism and superconductivity in $YBa_2(CuFe_x)_3O_4$ by magnetic susceptibility measurements. Loya et al [91], explained the behavior of antiferromagnets and superconductors in $SmRh_4B_4$. Singh et al [92], studied the possible relationship between superconductivity and antiferromagnetism in $EuBa_2Cu_3O_7$ high T_c superconductors. They found a distinct possibility of the coexistence of superconductivity and antiferromagnetic ordering. The nature of magnetic ordering in $HoNi_2B_2C$ and $ErNi_2B_2C$ has been clearly established by Chang et al [93] using neutron diffraction studies(NDS). As a result, antiferromagnetic ordering in $HoNi_2B_2C$ and ferromagnetic ordering in $ErNi_2B_2C$ has been found. Furthermore, it was found by Lee et al [94], that the temperature at which superconductivity sets in is same as where static internal magnetic field develops. The coexistence of superconductivity and magnetic ordering in different temperature ranges in some ternary compounds such as RRh_4B_4 and RMo_6S_8 is suggestive of a new mechanism of a transition from one phase to another. In the case of $ErRh_4B_4$, superconductivity sets in at T_{sc}=8.7K and localized magnetic moments start to align ferromagnetically at T_m= 1.2K. The superconductivity finally disappears at about 0.9K, thus there is a narrow temperature range in which superconductivity coexists with ferromagnetism.

A similar behavior is observed for the compound $Ho_{1.2}Mo_6S_8$ which becomes superconducting at 1.2K and returns to the normal state, but with magnetic ordering at 0.6 K[92]. Zang et al [95], measured magnetization as a function of temperature in single crystal $TlBa_2Ca_3Cu_4O_{11-\delta}$ and found linear temperature dependence for the reversible magnetization. It is believed that magnetism in copper oxides arises from the incomplete outer shells of the copper ions and the fluctuations in these unpaired spins give rise to collective magnetic excitations which are coherent over many lattice sites[96].

One of the most dramatic manifestation of the interaction between superconductivity and magnetism is the induction of superconductivity through the application of high magnetic field. It is found out that, magnetic field tends to enhance pairing fluctuations near the transition temperature. Jaccarino et al[97], predicted theoretically the induction of superconductivity by application of magnetic field. After some twenty years of their proposal, magnetic field superconductivity was established experimentally by Meul et al[98], in $Eu_xSn_{1-x}Mo_6S_8$ for ($x \simeq 0.8$).

Kebede et al[99], studied the magnetic thermal transport and structural properties of alloy $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$. They found that superconducting T_c is reduced by increasing Pr concentration. According to Abrikosov and Gorkov pair breaking mechanism with critical concentration(x_c =0.62), the alloying reduces the Ne'el temperature(T_N) linearly with Yttrium(Y) concentration region($0.4 < x < 0.6$) where antiferromagnetism and superconductivity is believed to coexist. Hirsch[45], showed on the assumption that doping creates holes on the oxygen rather than on the Cu sites and antiferromagnetic ordering of the Cu moments will lead to either localization or pairing of oxygen holes. It is further suggested that magnetic anisotropy strongly enhances superconductivity in the high T_c cuprates. Aoki et al[100], observed the dependence of T_c by substituting Cobalt(Co) in $YBa_2(Cu_{1-x}Co_x)_3O_y$. They measured T_c and magnetic susceptibility which depends upon the substitution of concentration. Lyubutin et al [101], found magnetically ordered states in the oxygen deficient $(Cu_{1-x}Fe)O_{y<6.5}$ system ($0.01 \leq\ x\ \leq 0.30$) using Mössbauer Spectroscopy. Kastner et al [102], indicated the dual nature of Copper(Cu) atoms. They found that by doping lanthanum cuprate with holes destroys antiferromagnetism and for higher concentration of holes superconductivity occurs. They argued that, as the dopant atoms are not replacing the magnetic ions, in this system the same atom that is, Cu is responsible for both phenomena. One of the attractions of quaternary borocarbide superconductors[76, 103, 104] is the coexistence of superconductivity and magnetism found in some of the members at relatively elevated temperature[105]. For instance, RNi_2B_2C(R=Tm, Er, Ho, and Dy) where($T_c \simeq$ 11K, 10 K, 8K, 6K, and $T_N \simeq$ 1.5K, 6K, 8K, 11K respectively) are magnetic superconductors. Amongst the other members of the family which contain magnetic ions, superconductivity has been observed in $PrPt_2B_2C$[73].

Magnetic superconductors have recently attracted growing interest with the discovery of the ferromagnetically ordered state coexisting with superconductivity in UGe_2[4], $URhGe$[5] and $ZrZn_2$[6]. Thus, it is important to study the interplay between magnetism and superconductivity in the case where the coupling between these subsystems is weak. A weak coupling between magnetic and conduction electrons is also required to explain the coexistence between superconductivity and long-range antiferromagnetic ordering at low temperatures[106]. A weak but non-negligible interaction between Gd 4f and Cu 3d electrons, possibly via modified oxygen 2p orbital has been verified through specific heat and inelastic magnetic scattering measurements[107]. For the superconducting $GdBa_2Cu_3O_{7-\delta}(Gd_{123})$, information pertaining to the antiferomagnetic transition of Gd^{3+} ions has been obtained from neutron scattering [108] and specific heat experiments[109]. It has been confirmed that long-range antiferromagnetism and superconducting ordering interact in $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$ with $\eta \leq 0.2$[110]. For the sample $Gd_{1.2}Ba_{1.8}Cu_3O_{7.03}$, T_c is decreased to 42K by the substitution of Gd on the Ba site while keeping the oxygen content as large as possible. For this sample, superconducting currents are unable to screen the antiferromagnetism fluctuations of the Gd^{3+} magnetic moments, and as a consequence a peak in the temperature dependence of the ac susceptibility is observed at T_N as shown in fig. 2.2. This proves that the coupling between the localized Gd 4f and the conduction Cu 3d and /or oxygen 2p electrons is sufficiently strong and results in the pair breaking effect due to the spin-disorder scattering.

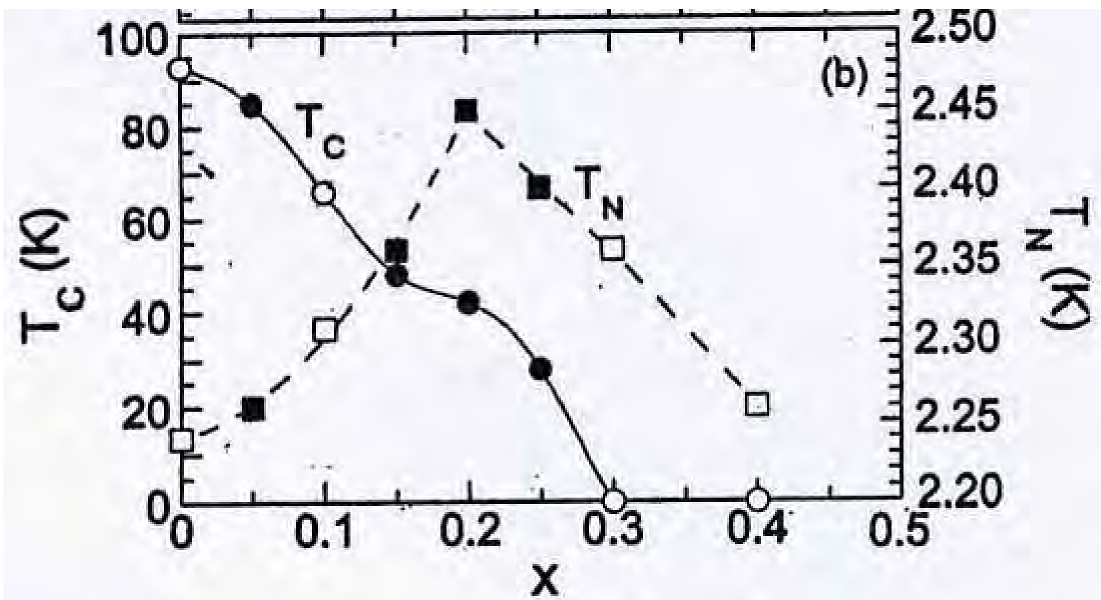

Fig. 2.2: Phase diagram of the superconducting transition temperature(T_c) and the antiferromagnetic ordering temperature(T_N) versus magnetic impurity(X)[110].

For the $Gd_{1.2}Ba_{1.8}Cu_3O_{7.03}$ compound, a clear peak in the real part of the ac susceptibility has been observed at $T_N = 2.45K$ and interpreted as a result of the conventional pair breaking effect enhanced close to the magnetic phase transition temperature. For the $Gd_{1.2}Ba_{1.8}Cu_3O_{7.03}$ compound in a magnetic field, T_N is remarkably different for the superconducting and the oxygen deficient non-superconducting sample. This observation together with the single anomaly in the temperature dependence of the real part of the ac susceptibility near T_N gives strong evidence that separation of the superconducting and the normal magnetic phases can be excluded. Thus, superconductivity and long- range antiferromagnetic ordering interact here as truly coexisting effects[110].

It is believed that in UGe_2, URhGe and $ZrZn_2$ compounds, ferromagnetism arises from a different type of electron pairing mechanisms. In these compounds, electrons with spins pointing in the same direction team up with each other to form Cooper pairs with one unit of spin resulting in triplet pairing superconductivity. In contrast, in the conventional theory, superconductivity occurs when electrons with opposite spins bind together to form the singlet state, that is, Cooper pairs with zero momentum and spin. The search for ferromagnetic superconductors goes back to the 1960s when superconducting materials with magnetic impurities were studied[77]. The search in this direction has led to the works of Larkin et al[111] and Fulde et al [112] who studied a simple model of effective field theory of superconducting fermions coupled to magnetic impurities and they described the phase diagram of such a system. In the recent discovery of superconducting ferromagnets - UGe_2 and $URhGe$, the electrons responsible for the ferromagnetic order are found to be the same as those which participate in the Cooper pair formation[4, 5]. Even though, superconductivity and ferromagnetism are thought to be basically mutually repulsive, Ginzburg[57] pointed out a possibility of their coexistence under the condition that the magnetization is less than the thermodynamic critical field(H_{c2}). In the rare - earth ternary compounds such as $HoMo_6S_8$ and $ErRh_4B_4$, the coexistence of ferromagnetism and superconductivity has been speculated below T_m[113].

Anderson et al[114], discussed the crypto-ferromagnetism as a possible coexistence phase where the ferromagnetism is modified to a long-period modulated spin structure. Recently, Saxena et al[4], found that superconductivity in polycrystalline ferromagnetic UGe_2 coexists up to 30K. Another study at Grenoble Research Center revealed that UGe_2 displays Meissner effect which is one of the hallmarks of superconductivity. The Grenoble group recently discovered that URhGe is a ferromagnetic superconductor at ambient pressure(p=0) while the coexistence of superconductivity and ferromagnetism in UGe_2 is realized at a pressure of about 16kbar. Correlation of superconductivity and magnetism has been one of the central issues in the field of strongly correlated electron systems. In particular, one may find interesting materials showing the coexistence of superconductivity with ferromagnetic or antiferromagnetic ordering in uranium based intermetallic compounds. These materials contain a periodic array of uranium ions[115]. It is well known that the series of rare earth rhodium borides exhibit the coexistence of superconductivity and magnetism[89]. Thorough investigation on the systems revealed that magnetism is carried by 4f electrons well localized on rare earth atom sites of Er and the superconductivity by 4d electrons of Rh atoms in $ErRh_4B_4$ which implies that superconductivity and ferromagnetism are separated in real space. However, uranium based compounds such as UPd_2Al_3, UNi_2Al_3, URu_2Si_2 and UGe_2 show quite a different kind of coexistence. The electrons responsible for the ferromagnetic order are found to be the same as those which participate in the Cooper pairs. That is, both magnetism and superconductivity are carried by uranium 5f- electrons. Polarized neutron scattering experiments revealed that, the localized magnetic moments are sitting on uranium ion sites[89] whereas, a specific heat jump at the superconducting transition temperatures($T_c \simeq 2K$) is comparable to a value predicted from the BCS theory, the latter fact indicating that heavy quasi-particles originating from 5f electrons carry superconducting currents. UNi_2Al_3 exhibits the coexistence of superconductivity at $T_c \simeq 1K$ and antiferromagnetism at $T_N \simeq 4K$ [116]. In ferromagnetic materials such as UGe_2, the superconducting electrons detect a non-vanishing internal field. Thus, ferromagnetism with a local moment of the order of $1\frac{\mu_B}{U}$(μ_B being the Bohr magneton) coexists with superconductivity in UGe_2.

2.3.1 Pressure Induced Superconductivity And Ferromagnetism In UGe_2

As was stated earlier UGe_2[4], URhGe[5] and $ZrZn_2$[6] are the recently discovered ferromagnetic superconductors. Although superconductivity and ferromagnetism have been established to occur in several materials, UGe_2 represented the first example where ferromagnetism and superconductivity are not competing orders but coexisting simultaneously[4,117]. The magnetic moments of these uranium based superconductors which originate from uranium 5f-electrons are too large and too ordered to foster strong magnetic fluctuations. The main reason for this is their behavior to pressure. It is well known that, when a material is compressed by the application of high pressure, the atoms are pushed closer together, making it easier for the electrons to hop from one atomic site to another. This enables to broaden the energy bands of the material. Since broad bands do not favor magnetism, pressure almost universally tends to make the Curie temperature(T_m) to go down and eventually vanishes at the critical pressure(P_c)[4,117]. In the case of UGe_2, URhGe and other f-band systems, the conduction bands are rather narrow. Squeezing f-band systems give experimenters ample space to explore a wide range of electronic states that might support coexistence of ferromagnetism and superconductivity in these materials.

It is noteworthy that, the superconductivity in UGe_2 disappears above a critical pressure(P_c) of about 16kbar beyond which ferromagnetism is suppressed. This fact implies that superconductivity and ferromagnetism in UGe_2 may be cooperative phenomena. It is, however, currently believed that the uniformly coexistent phase of ferromagnetism and superconductivity is unlikely to exist since the Cooper pairs feel a non-vanishing internal field to prevent the onset of a spin-singlet superconductivity. It is therefore, surprising that both ferromagnetism and superconductivity are carried by 5f-electrons of uranium atoms and the superconductivity coexists with ferromagnetism with a large moment of the order of $1\mu_B/U$ which suggests that a spin-triplet pairing state may be formed. This indicates that, the uranium 5f-electrons have dual nature, that is, they are responsible of producing both superconductivity and ferromagnetism. On the other hand, superconductivity and ferromagnetism have been reported in $HoMo_6S_8$[56], $ErRh_4B_4$[118] and $ErNi_2B_2$[119]. However, in these systems $T_m < T_{sc}$ and the superconducting and ferromagnetic orders are competing. In these materials, the ferromagnetism is carried by localized 4f electrons of Ho and Er atoms, whereas the superconductivity is carried by the conduction electrons. As can be seen from the temperature versus pressure phase diagram of UGe_2 given in fig.2.3, the Curie temperature(T_m) of UGe_2 decreases monotonically from T_m=52K at zero pressure with increasing pressure. Moreover, a characteristic transition temperature(T^*) is observed below T_m which decreases monotonically with pressure as T_m does. Both T_m and T^* decrease approximately as a function of $(P_c - P)^n$ (where, n $\simeq$ 0.5 - 0.4)[120].

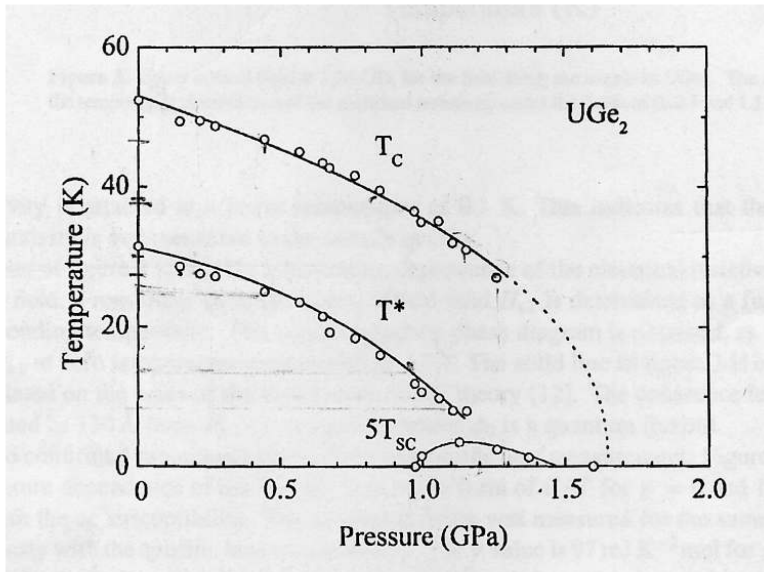

Fig. 2.3: Temperature versus pressure phase diagram of UGe_2. Superconductivity is observed in a narrow region just within the ferromagnetic state of an itinerant electron system[120].

T^* is observed at about 30K and it becomes close to zero at a pressure of 12kbar, where the superconductivity transition temperature is about T_{sc}=0.7K[4]. Superconductivity sets in at a pressure of about 10kbar exhibiting a maximum value of superconducting temperature, $T_{sc} = 0.7k$ around a pressure of 12kbar[121]. The superconductivity in UGe_2 disappears above a pressure of about 16kbar which coincides with the pressure at which the ferromagnetism is suppressed. The fact that both superconductivity and magnetism disappear simultaneously in UGe_2 at P_m=16kbar suggests that superconductivity is in spin triplet pairing state under the background of ferromagnetism and both superconductivity and ferromagnetism are in cooperative phenomenon in UGe_2[121].

2.3.2 Overview Of The Properties Of $GdBa_2Cu_3O_{7-\delta}$

The superconducting phase in all the cuprates has common features. They are all type II superconductors. Most of the high T_c superconducting materials are layered cuprates. That is, they consist of CuO_2 planes separated by layers of other oxide elements. $GdBa_2Cu_3O_{7-\delta}$ is a hole doped cuprate which has a perovskite type crystal structure. $GdBa_2Cu_3O_{7-\delta}$ is a highly anisotropic material, that is, the value of superconducting parameter is different in different directions and the charge transport is mainly confined to the copper oxide planes.

Detailed studies on the role of oxygen content have not been reported so far for Gd compounds such as $GdBa_2Cu_3O_{7-\delta}$, but in view of the overall similarity found for analogous compounds with Yttrium(Y) and rare-earth elements such as Gd, the same behavior is expected for Gd compounds as well[122]. Which means that, the replacement of Y by other rare-earth elements cause no appreciable change in the superconducting properties. Therefore, the properties and crystal structure of $GdBa_2Cu_3O_{7-\delta}$ is considered to be similar to $YBaCu_2O_{7-\delta}$. The properties of $GdBa_2Cu_3O_{7-\delta}$ depend upon the oxygen content δ. For small values of δ ($\delta \simeq 0$), the lattice structure is perfectly ordered and is in the orthorhombic phase, that is, a$\neq$ b$\neq$ c, α=β=γ=90^0. The orthorhombic phase is the superconducting state and the transition to superconducting state occurs above 90K for $\delta \leq 0.2$[123]. The superconducting transition temperature decreases with increasing the oxygen deficiency(δ). For $\delta > 0.5$, the crystal symmetry of GBCO is reported to be tetragonal at low temperature, that is a=b$\neq$c, α=β=γ=90^0 and no transition to a superconducting state has been observed[106]. These changes are ascribed to a varying occupation of oxygen sites in Cu-O-Cu-O... chains with Cu(1) ions along the crystallographic b-axis. The distance Cu-O in the chains is about 1.9$\mathring{A}$, as that in the planes. These chains are thought to play a crucial role in the superconductivity in these compounds[124].

In high T_c superconductors such as $GdBa_2Co_3O_{7-\delta}(Gd_{123})$ the critical magnetic field(H_c) is large enough($80T < H_c < 180T$) to be studied at temperatures where the long range antiferromagnetic ordering of the rare-earth ions appear. The dimensions of the single unit cell GBCO are $a = 3.82\mathring{A}$, $b = 3.89\mathring{A}$ and $c = 11.68\mathring{A}$. Besides, $\lambda_L = 1450\mathring{A}$ and $\xi = 130\mathring{A}$. Superconductivity is thought to be constrained to lattice planes formed essentially by copper and oxygen ions. The planes containing Gd are well separated by about $6\mathring{A}$ from the superconducting layer[122] as shown in fig.2.4. The figure shows the layered structure of $GdBa_2Cu_3O_{7-\delta}$ superconductor. The unit cell crystal structure of $GdBa_2Cu_3O_{7-\delta}$ consists of two CuO_2 planes separated by Gd atoms. The intercalating layers separating these double CuO_2 planes contain the Cu, Barium(Ba) and O_2 atoms. Thus, superconductivity and magnetism should coexist perfectly in these compounds. This expectation has been substantiated by investigations of the magnetic properties of $GdBa_2Cu_3O_{7-\delta}$. Furthermore, in $GdBa_2Cu_3O_{7-\delta}$, Gd is the only magnetic species and no magnetic moments reside on Cu ions[122].

For the layered structure with Gd-Gd distances of $\sim 3.8\mathring{A}$ within(a,b) planes and inter-planar Gd-Gd distances near $12\mathring{A}$, a largely two dimensional character of the magnetic ordering may be expected as well. A natural model that arises from the common structural features of the copper oxide superconductors is that the superconductivity occurs predominantly in the CuO_2 planes, while the intercalated layers provide in some fashion, carriers or the coupling mechanism necessary for superconductivity. Based on this hypothesis, it is instructive to view the layered copper oxide superconducting compounds as consisting of CuO_2 layers and charge

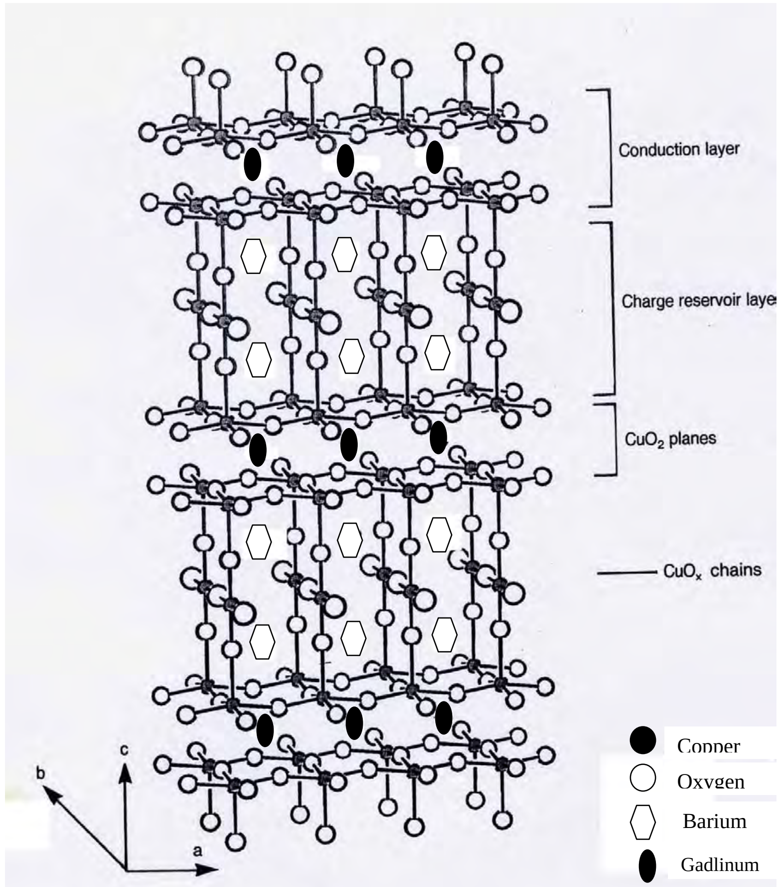

Fig. 2.4: The unit cell crystal structure of $GdBa_2Cu_3O_{7-\delta}$.

reservoir or intercalated layer as shown in fig 2.4. Such models are known as charge transfer models[125]. The number of carriers in the conduction layer is controlled by the amount of charges transferred between the conduction layer and the charge reservoir layer.

2.3.3 Overview Of The Properties Of UGe_2

The crystal structure of UGe_2 is an orthorhombic(space group C_{mmm}) type and contains zigzag chains of nearest-neighbor uranium ions. In UGe_2 the nearest-neighbor

U distance (d_{u-u})) is 3.85$\AA$ at ambient pressure, but this is plausibly reduced to $d_{u-u} = 3.5\AA$ at a pressure of 13kbar. Thus, pressure increases the extent of delocalization of the f-electrons as d_{u-u} is decreased. This offers a possible mechanism to explain the suppression of the Curie temperature(T_m) with pressure. Apart from separating the uranium atoms it should be remembered that the Germanium(Ge) atoms might also play a second role in hybridizing with the uranium($d_{u-Ge} = 2.9\AA$). The increase in uranium separation leads to a greater localization of the f-electrons and much larger magnetic entropy at low temperature.

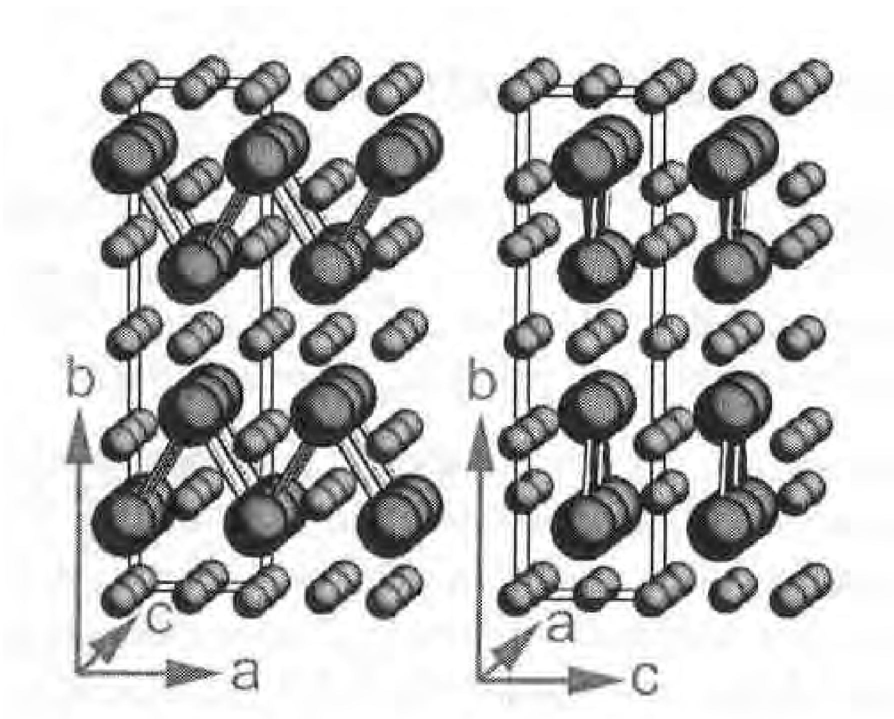

Fig. 2.5: The crystal structure of UGe_2 is shown above. Thick bars connect nearest neighbor atoms(large spheres) that form zigzag chains parallel to the crystal a-axis(the easy magnetization direction). The Ge atoms are shown as small spheres and the orthorhombic unit cell by the fine lines[126].

The essential fact relevant to spin-triplet superconductivity is that UGe_2 is intrinsically structurally ordered material. The inherent anisotropy due to the uranium 5f-electron is further emphasized by the choice of a base-centered orthorhombic crystal structure and space group of C_{mmm} with lattice spacing of a=4.0089$\AA$, b=15.0889$\AA$ and c=4.0950$\AA$)[126] as shown in fig. 2.5.

As mentioned earlier, the uranium atoms in UGe_2 are arranged as zigzag chains of nearest neighbors that run along the crystallographic a-axis which is the easy magnetic direction and lying within a-b plane. However, inter-chain and intra-chain separations are comparable and each U is tenfold coordinated by UGe_2.

3. MATHEMATICAL TECHNIQUE

In the present work, we have used double time temperature dependent Green's function technique, Zubarev[127], to study the problem of the coexistence of superconductivity and magnetism in $GdBa_2Cu_3O_{7-\delta}$ and UGe_2. The concept of Green's function originated with the work of Green in potential theory. Green's work which was primarily concerned with the study of methods of solving Laplace's and Poisson's equations with the various boundary conditions contained the germs of a much wider application for solving a variety of eigenvalue problems of linear operators such as annihilation and creation operators and the corresponding inhomogeneous equations. The Green functions are the appropriate generalization of the concepts of correlation functions and work as propagators. They are connected with the evaluation of observed quantities and they have well known advantages when quantities are formulated and solved. We can consider in quantum field theory(QFT) the different kinds of Green functions such as the double time causal, retarded and advanced Green functions which are defined respectively by,

$$G_c(t-t') = \langle\langle \hat{A}(t), \hat{B}(t')\rangle\rangle_c = -i\langle T\hat{A}(t)\ \hat{B}(t')\rangle \tag{3.1}$$

$$G_r(t-t') = \langle\langle \hat{A}(t), \hat{B}(t')\rangle\rangle_r = -i\Theta(t-t')\langle\left[\hat{A}(t)\ \hat{B}(t')\right]\rangle \tag{3.2}$$

$$G_a(t-t') = \langle\langle \hat{A}(t), \hat{B}(t')\rangle\rangle_a = i\Theta(t'-t)\langle\left[\hat{A}(t)\hat{B}(t')\right]\rangle \tag{3.3}$$

where $\langle\langle \hat{A}(t), \hat{B}(t')\rangle\rangle_{c,r,a}$ are abbreviated notations for the corresponding Green functions and $\langle \quad \rangle$ indicates the average over a grand canonical ensemble for any operators. $\Theta(t-t')$ is Heaviside step function, A(t) and B(t') are the Heisenberg representations of the operators $\hat{A}$ and $\hat{B}$ expressed in terms of a product of quantized field functions or particle creation and annihilation operators expressed by,

$$\hat{A}(t) = \exp(i\varrho t)\hat{A}\exp(-i\varrho t) \tag{3.4}$$

where $\varrho = \hat{H} - \mu N$ and μ is the chemical potential.

The symbol T indicates the time ordered or T product of operators which is defined by,

$$T\hat{A}(t)\hat{B}(t') = \Theta(t-t')\hat{A}(t)\hat{B}(t') + \nu\Theta(t'-t)\hat{B}(t')\hat{A}(t) \tag{3.5}$$

where

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

The expression $\left[\hat{A}(t),\ \hat{B}(t')\right]_{\mp}$ indicates the commutator or anti-commutator which is expressed by

$$\left[\hat{A}(t)\ \hat{B}(t)\right]_{\mp} = \hat{A}(t), \hat{B}(t') \mp \nu\hat{B}(t')\hat{A}(t) \tag{3.6}$$

where $\nu = 1$, for Bosons and $\nu = -1$, for Fermions.

Which means that for two boson operators,

$$[\hat{A}_{k\sigma}, \hat{A}^{\dagger}_{k'\sigma'}]_{-} = \hat{A}_{k\sigma}\hat{A}^{\dagger}_{k'\sigma'} - \hat{A}^{\dagger}_{k'\sigma'}\hat{A}_{k\sigma} = \delta_{kk'}\delta_{\sigma\sigma'} \tag{3.7}$$

and

$$[\hat{A}_{k\sigma}, \hat{A}_{k'\sigma'}]_{-} = [\hat{A}^{\dagger}_{k\sigma}, \hat{A}^{\dagger}_{k'\sigma'}]_{-} = 0 \tag{3.8}$$

Similarly, for two Fermion operators, we have

$$[\hat{A}_{k\sigma}, \hat{A}^{\dagger}_{k'\sigma'}]_{+} = \hat{A}_{k\sigma}\hat{A}^{\dagger}_{k'\sigma'} + \hat{A}^{\dagger}_{k'\sigma'}\hat{A}_{k\sigma} = \delta_{kk'}\delta_{\sigma\sigma'} \tag{3.9}$$

and

$$[\hat{A}_{k\sigma}, \hat{A}_{k'\sigma'}]_{+} = [\hat{A}^{\dagger}_{k\sigma}, \hat{A}^{\dagger}_{k'\sigma'}]_{+} = 0 \tag{3.10}$$

In this work, we confine ourselves to retarded double time temperature dependent Green's function since it implies the principle of causality.

In order to obtain the equation of motion for the Green's function, we differentiate eq.(3.2) with respect to time and obtain,

$$\frac{dG_r(t-t')}{dt} = \frac{d}{dt}\langle\langle \hat{A}(t), \hat{B}(t')\rangle\rangle$$

$$\Longrightarrow \frac{dG_r(t-t')}{dt} = -\frac{d}{dt}\Big[i\Theta(t-t')\langle[\hat{A}(t)\ \hat{B}(t')\Big]\rangle$$

$$\Longrightarrow \frac{dG_r(t-t')}{dt} = -i\frac{d}{dt}\Theta(t-t')\langle\Big[\hat{A}(t)\ \hat{B}(t')\Big]\rangle - i\Theta(t-t')\langle\left[\frac{d\hat{A}(t)}{dt}\hat{B}(t')\right]\rangle \tag{3.11}$$

Multiplying both sides of eq.(3.11) by "i", we obtain

$$i\frac{dG_r(t-t')}{dt} = \frac{d}{dt}\Theta(t-t')\langle\Big[\hat{A}(t)\hat{B}(t')\Big]\rangle - i\Theta(t-t')\langle[i\frac{d\hat{A}(t)}{dt}\hat{B}(t')]\rangle \tag{3.12}$$

Using the notation

$$i\frac{dG_r(t,t')}{dt} = i\dot{G}(t-t')$$

eq.(3.12) becomes,

$$i\dot{G}(t-t') = \frac{d}{dt}\Theta(t-t')\langle\Big[\hat{A}(t)\hat{B}(t')\Big]\rangle + \langle\left[i\frac{d\hat{A}(t)}{dt}\hat{B}(t')\right]\rangle \tag{3.13}$$

Employing the relation between Heaviside step function $\Theta(t)$ and $\delta(t)$ such that

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

and the equation of motion,

$$i\frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t)\ \hat{H}\right]$$

where, $\hbar$=1

the equation of motion for the Green function $\dot{G}_r(t,t')$ given in eq.(3.13) can be expressed by,

$$\dot{G}_r(t,t') = \frac{d}{dt}\Theta(t-t')\langle\left[\hat{A}(t)\ \hat{B}(t')\right]\rangle + \langle\langle\left[\hat{A}(t)\ \hat{H}\right], \hat{B}(t')\rangle\rangle$$

which implies that,

$$i\dot{G}_r(t-t') = \delta(t-t')\langle\left[\hat{A}(t), \hat{B}(t')\right]\rangle + \langle\langle\left[\hat{A}(t)\ \hat{H}\right], \hat{B}(t')\rangle\rangle \tag{3.14}$$

To solve eq.(3.14), it is convenient to work with Fourier transformation of this equation. A careful analysis shows that the function depends on time t and t' through(t-t'). Thus we can write, $G_r(t-t') = G_r(t'-t)$.

Now, let $G_r(\omega)$ be the Fourier transformation of $G_r(t-t')$ such that

$$G_r(t-t') = \int_{-\infty}^{\infty} G_r(\omega)e^{-i\omega(t-t')}d\omega \tag{3.15}$$

and

$$G_r(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G_r(t-t')e^{i\omega(t-t')}dt \tag{3.16}$$

From the analytical property of $G_r(\omega)$ we have

$$\langle\hat{B}(t')\ \hat{A}(t)\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} \Im\frac{G_r(\omega+i\epsilon)}{e^{\beta\omega}+1}dt \tag{3.17}$$

and using the definition of the δ-function given by,

$$\delta(t-t') = \int_{-\infty}^{\infty} e^{-i\omega(t-t')} d\omega \tag{3.18}$$

eq.(3.14) can be transformed to the following expression,

$$\omega G_r(\omega) = \langle \left[\hat{A}(t)\ \hat{B}(t') \right] \rangle + \langle\langle \left[\hat{A}(t)\ \hat{H} \right], \hat{B}(t') \rangle\rangle_\omega \tag{3.19}$$

where, $\langle\langle \quad \rangle\rangle_\omega$ stands for the Fourier transformation of the corresponding Green's function. The correlation function $\langle \hat{B}(t')\hat{A}(t) \rangle$ is related to the Green's function by,

$$\langle \hat{B}(t')\hat{A}(t) \rangle = i \lim_{\epsilon \longrightarrow 0} \int_{-\infty}^{\infty} \frac{\left[\langle\langle \hat{A}, \hat{B} \rangle\rangle_{\omega+i\epsilon} - \langle\langle \hat{A}, \hat{B} \rangle\rangle_{\omega-i\epsilon} \right] e^{i\omega(t-t')} d\omega}{e^{\beta\omega} + \nu} \tag{3.20}$$

where, $\beta = \frac{1}{\kappa_B T}$ and κ_B is the Boltzmann constant.

The other standard relation used to calculate correlation function is given by

$$\frac{1}{E - \omega \pm i\epsilon} = \frac{P}{E - \omega} \mp i\pi\delta(E - \omega) \tag{3.21}$$

where $\epsilon > 0$ and P denotes the principal value of the integral. Here, we consider $E - \omega$ as a real quantity.

In order to obtain the superconducting properties, we define the following correlations in our formalism,

$$\Delta = V \sum_k \langle \hat{a}^\dagger_{-k\downarrow} \hat{a}^\dagger_{k\uparrow} \rangle = \sum_k V \langle \hat{a}_{-k\downarrow} \hat{a}_{k\uparrow} \rangle \tag{3.22}$$

The superconducting order parameter(Δ) can be found from the correlation function $\langle\ \hat{a}_{-k\downarrow}\hat{a}_{k\uparrow} \rangle$ and/ or $\langle \hat{a}^\dagger_{k\uparrow}\hat{a}^\dagger_{-k\downarrow} \rangle$ using eq.(3.20) with the appropriate Hamiltonian.

By letting $\Delta \longrightarrow 0$ as T $\longrightarrow T_c$, we get the expression for T_c as,

$$\kappa_B T_c = 1.14\ \hbar\omega_b \exp(-\frac{1}{\lambda}) \tag{3.23}$$

where $\lambda =$ VN(0)

4. FORMULATION OF THE PROBLEM

4.1 Coexistence of Superconductivity And Antiferromagnetism In $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$

4.1.1 *Introduction*

The recent discovery of the coexistence of superconductivity and antiferromagnetism for the first time in high T_c superconductors such as $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$ is a remarkable development. Experimental studies have revealed the coexistence of superconductivity and antiferromagnetism and the variation of the superconducting transition temperature (T_c) with magnetic ordering(η)[109]. Following the experimental observations, a theoretical study has been made by considering a model Hamiltonian consisting of a pairing interaction, intra and inter atomic Coulomb interactions, exchange interactions and scattering of Cooper pairs by magnetic moments(or spins) of gadolinium(Gd)ions. $GdBa_2Cu_3O_{7-\delta}$ is a highly anisotropic compound, that is, the value of superconducting parameters are different at different directions and the charge transport is mainly confined to CuO_2 planes. The properties of $GdBa_2Cu_3O_{7-\delta}$ depend upon the oxygen content(δ). For small values of δ, the lattice structure is perfectly ordered and is in the orthorhombic phase and a transition to superconducting state occurs above 90K for $\delta \leq 0.2$.

In high T_c superconductors such as $GdBa_2Cu_3O_{7-\delta}(Gd_{123})$, the critical magnetic field (H_c) is large to be studied at temperatures where the long range antiferromagnetic ordering of the rare earth ions appear. Superconductivity in $GdBa_2Cu_3O_{7-\delta}$ is thought to be constrained to planes formed essentially by copper and oxygen ions. The planes containing Gd are well separated by about $6\mathring{A}$ from the superconducting layer[122]. The unit cell crystal structure of $GdBa_2Cu_3O_{7-\delta}$ contains two CuO_2 planes separated by Gd atoms. The intercalating layers separating these double CuO_2 planes contain the Cu, Ba and O_2 atoms. Thus, superconductivity and antiferromagnetism coexist perfectly in $GdBa_2Cu_3O_{7-\delta}$. This expectation has been substantiated by investigations of the magnetic properties of $GdBa_2Cu_3O_{7-\delta}$. Experimental findings have confirmed that, in $GdBa_2Cu_3O_{7-\delta}$ the magnetism is due to the 4f electrons associated with Gd ions and not due to the Cu ions[122].

Using the double time temperature dependent Green's function formalism and appropriate decoupling approximations, the coexistence of superconductivity and antiferromagnetism has been shown to be a very distinct possibility. In this section, we investigate the coexistence of superconductivity and antiferromagnetism in $GdBa_2Cu_3O_{7-\delta}$ and the effect of magnetic ordering on both the superconducting order parameter(Δ) and the transition temperature(T_c).

4.2 Mathematical Formulation Of The Problem

The model Hamiltonian for our system can be described as follows

$$\hat{H} = \sum_{k,\sigma} \epsilon_k \hat{a}^\dagger_{k\sigma}\hat{a}_{k\sigma} - \sum_{k,k'} V_{kk'}\hat{a}^\dagger_{k\uparrow}\hat{a}^\dagger_{-k\downarrow}\hat{a}_{-k'\downarrow}\hat{a}_{k'\uparrow} + \sum_{n,\sigma} E_n b^\dagger_{n\sigma}b_{n\sigma} + \sum_{nm\sigma\sigma'} J_{nm} b^\dagger_{n\sigma}b^\dagger_{m\sigma'}b_{m\sigma'}bn\sigma$$

$$+U\sum_{\ell} n_{\ell\uparrow}n_{\ell\downarrow} + U'\sum_{\ell\ell'\sigma\sigma'} n_{\ell\sigma}n_{\ell'\sigma'} + \sum_{k\ell m}\Omega^{\ell m}_k (b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}\hat{a}_{k\downarrow}\hat{a}_{-k\uparrow} + h.c) \tag{4.2.1}$$

where $\hat{a}^\dagger_{k\sigma}(\hat{a}_{k\sigma})$ denote the fermion creation (annihilation) operator, $\mathbf{k}$ and σ are the wave vector and the spin index. ϵ_k and V are respectively the kinetic energy of the free charge carriers and the usual BCS type of pairing interaction resulting from bosonic exchange, $b^\dagger_{n\sigma}(b_{n\sigma})$ denote the creation(annihilation) of electrons with spin σ at the localized site, E_n is the energy of the localized electrons, J_{nm} denotes the exchange interaction between localized electrons. The fifth and sixth terms represent the intra and inter atomic interactions respectively. The last term describes the interaction between the scattering of Cooper pairs by localized antiferromagnetic electrons[128]. We study the problem in the sprit of BCS theory with unspecified mechanism of superconductivity till the matter is settled with regard to pairing interaction[129].

In order to obtain the self consistent expression for the superconducting order parameter as a function of the magnetic ordering(η), we apply the Green's function formalism.

Defining

$G^{\uparrow\uparrow}_{kk'} = \langle\langle \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k'\uparrow}\rangle\rangle$

and writing equation of motion

$$\omega\langle\langle \hat{a}_{k\uparrow}, \hat{a}^\dagger_{k'\uparrow}\rangle\rangle = \frac{\delta_{kk'}}{2\pi} + \langle\langle \left[\hat{a}_{k\uparrow}\hat{H}\right], \hat{a}^\dagger_{k'\uparrow}\rangle\rangle \tag{4.2.2}$$

Evaluating the commutator using the Hamiltonian given in eq.(4.2.1), we obtain

$$\left[\hat{a}_{k\uparrow}, \sum_{p,\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}\right] = \sum_{p,\sigma} \epsilon_p \left[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}\right]_- = \epsilon_k \hat{a}_{k\uparrow} \tag{4.2.3}$$

$$\begin{aligned}\left[\hat{a}_{k\uparrow}, V\sum_{p,p'} \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}\right] &= V\sum_{p,p'} \left[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}\right]_+ \\ = V\sum_{p,p'}\{[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}]\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow} &+ \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}[\hat{a}_{k\uparrow}, \hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}]\} \\ &= V\sum_{p,p'}\{[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow}]\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow} + 0\} \\ &= V\sum_{p'} \hat{a}^{\dagger}_{-k\downarrow}\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}\end{aligned} \tag{4.2.4}$$

$$\left[\hat{a}_{k\uparrow}, \sum_{n,\sigma} E_n b^{\dagger}_{n\sigma}b_{n\sigma}\right] = \sum_{n,\sigma} E_n \left[\hat{a}_{k\uparrow}, b^{\dagger}_{n\sigma}b_{n\sigma}\right]_- = 0 \tag{4.2.5}$$

$$\left[\hat{a}_{k\uparrow}, \sum_{nm\sigma\sigma'} J_{nm} b^{\dagger}_{n\sigma}b^{\dagger}_{m\sigma'}b_{m\sigma'}b_{n\sigma}\right] = \sum_{nm\sigma\sigma'} J_{nm} \left[\hat{a}_{k\uparrow}, b^{\dagger}_{n\sigma}b^{\dagger}_{m\sigma'}b_{m\sigma'}b_{n\sigma}\right]_+ = 0 \tag{4.2.6}$$

$$\left[\hat{a}_{k\uparrow}, U\sum_{\ell} n_{\ell\uparrow}n_{\ell\downarrow}\right] = U\sum_{\ell} \left[\hat{a}_{k\uparrow}, b^{\dagger}_{\ell\uparrow}b_{\ell\uparrow}b^{\dagger}_{\ell\downarrow}b_{\ell\downarrow}\right]_+ = 0 \tag{4.2.7}$$

Similarly,

$$\left[\hat{a}_{k\uparrow}, U'\sum_{\ell\ell'\sigma\sigma'} n_{\ell\sigma}n_{\ell'\sigma'}\right] = U'\sum_{\ell\ell'\sigma\sigma'} \left[\hat{a}_{k\uparrow}, b^{\dagger}_{\ell\sigma}b_{\ell\sigma}b^{\dagger}_{\ell'\sigma'}b_{\ell'\sigma'}\right]_+ = 0 \tag{4.2.8}$$

where $\langle n_{\ell\sigma}\rangle = \langle b^{\dagger}_{\ell\uparrow}b_{\ell\uparrow}\rangle$, $\langle n_{\ell\sigma'}\rangle = \langle b^{\dagger}_{\ell\downarrow}b_{\ell\downarrow}\rangle$, $\sigma = \uparrow$ and $\sigma' = \downarrow$

$$\left[\hat{a}_{k\uparrow}, \sum_{\ell mp} \Omega^{\ell m}_p b^{\dagger}_{\ell\uparrow}b^{\dagger}_{m\downarrow}\hat{a}_{p\downarrow}\hat{a}_{-p\uparrow}\right] = \sum_{\ell mp} \Omega^{\ell m}_p \left[\hat{a}_{k\uparrow}, b^{\dagger}_{\ell\uparrow}b^{\dagger}_{m\downarrow}\hat{a}_{p\downarrow}\hat{a}_{-p\uparrow}\right]_+ = 0 \tag{4.2.9}$$

$$\begin{aligned}\left[\hat{a}_{k\uparrow}, \sum_{\ell mp} \Omega^{\ell m}_p b_{m\downarrow}b_{\ell\uparrow}\hat{a}^{\dagger}_{-p\uparrow}\hat{a}^{\dagger}_{p\downarrow}\right] &= \sum_{\ell mp} \Omega^{\ell m}_p \left[\hat{a}_{k\uparrow}, b_{m\downarrow}b_{\ell\uparrow}\hat{a}^{\dagger}_{-p\uparrow}\hat{a}^{\dagger}_{p\downarrow}\right]_+ \\ \sum_{\ell mp} \Omega^{\ell m}_p\{[\hat{a}_{k\uparrow}, b_{m\downarrow}b_{\ell\uparrow}]\hat{a}^{\dagger}_{-p\uparrow}\hat{a}^{\dagger}_{p\downarrow} &+ b_{m\downarrow}b_{\ell\uparrow}[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{-p\uparrow}\hat{a}^{\dagger}_{p\downarrow}]\} \\ &= \sum_{\ell mp} \Omega^{\ell m}_p\{0 + b_{m\downarrow}b_{\ell\uparrow}[\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{-p\uparrow}\hat{a}^{\dagger}_{p\downarrow}]\} \\ &= \sum_{\ell,m} \Omega^{\ell m}_{-k} b_{m\downarrow}b_{\ell\uparrow}\hat{a}^{\dagger}_{-k\downarrow}\end{aligned} \tag{4.2.10}$$

Substituting eqs.(4.2.3 - 4.2.10) into eq.(4.2.2) for $[\hat{a}_{k\uparrow}\hat{H}]$, we get

$$\omega\langle\langle\hat{a}_{k\uparrow}\hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle_{\omega} = \frac{\delta_{kk'}}{2\pi} + \epsilon_k\langle\langle\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle - V\sum_{p'}\langle\langle\hat{a}^{\dagger}_{-k\downarrow}\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow},\ \hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle$$

$$+\sum_{\ell,m}\Omega^{lm}_{-k}\langle\langle b_{m\downarrow}b_{l\uparrow}\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle \tag{4.2.11}$$

Eq.(4.2.11) is linearized by decoupling the higher order Green's function into lower order by employing mean field decoupling approximation. Hence we get,

$$\langle\langle\hat{a}^{\dagger}_{-k\downarrow}\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}\hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle = \langle\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}\rangle\langle\langle\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle \tag{4.2.12a}$$

$$\langle\langle b_{m\downarrow}, b_{\ell\uparrow}\hat{a}^{\dagger}_{-k\downarrow}\hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle = \langle b_{m\downarrow}b_{\ell\uparrow}\rangle\langle\langle\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle \tag{4.2.12b}$$

Substituting eqs.(4.2.12a) and (4.2.12b) into eq.(4.2.11), we get

$$\omega\langle\langle\hat{a}_{k\uparrow}\hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle_{\omega} = \frac{\delta_{kk'}}{2\pi} + \epsilon_k\langle\langle\hat{a}_{k\uparrow}\hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle - V\sum_{p'}\langle\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}\rangle\langle\langle, \hat{a}^{\dagger}_{-k\downarrow}\hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle$$

$$+\sum_{\ell,m}\Omega^{\ell m}_{-k}\langle b_{m\downarrow}b_{\ell\uparrow}\rangle\langle\langle, \hat{a}^{\dagger}_{-k\downarrow}\hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle$$

$$(\omega-\epsilon_k)\langle\langle\hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle_{\omega} = \frac{\delta_{kk'}}{2\pi} - \Delta\langle\langle\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle + \eta\langle\langle\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k'\uparrow}\rangle\rangle$$

For k=k', we have

$$(\omega-\epsilon_k)\langle\langle\hat{a}_{k\uparrow}\hat{a}^{\dagger}_{k\uparrow}\rangle\rangle_{\omega} = \frac{1}{2\pi} - (\Delta-\eta)\langle\langle\hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k\uparrow}\rangle\rangle \tag{4.2.13}$$

where

$$\Delta = V\sum_{p'}\langle\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}\rangle$$

and

$$\eta = \sum_{\ell mk}\Omega^{lm}_{-k}\langle b_{m\downarrow}b_{\ell\uparrow}\rangle$$

Here, η describes the antiferromagnetic correlation amongst neighboring atomic sites with local magnetic moments.

Similarly, the equation of motion for the higher order Green's function $\langle\langle \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k\uparrow}\rangle\rangle$ can be obtained by evaluating the relevant commutators as shown below.

$$\omega\langle\langle \hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{k'\uparrow}\rangle\rangle_\omega = \langle\langle \left[\hat{a}^\dagger_{-k\downarrow}\ \hat{H}\right], \hat{a}^\dagger_{k'\uparrow}\rangle\rangle_\omega \tag{4.2.14}$$

$$\left[\hat{a}^\dagger_{-k\downarrow}\ \sum_{p,\sigma} \epsilon_p\ \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}\right] = \sum_{p,\sigma} \epsilon_p \left[\hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}\right]_- = -\epsilon_{-k}\hat{a}^\dagger_{-k\downarrow} \tag{4.2.15}$$

$$\left[\hat{a}^\dagger_{-k\downarrow}, V\sum_{p,p'} \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}\right] = V\sum_{p,p'} \left[\hat{a}^\dagger_{-k\downarrow},\ \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}\right]_+$$

$$= V\sum_{p,p'}\{[\hat{a}^\dagger_{-k\downarrow}, \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}]\hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow} + \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}]\}$$

$$= V\sum_{p,p'}\{[0 + \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{-p'\downarrow}\hat{a}_{p'\uparrow}]\}$$

$$= V\sum_{p} \hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{k\uparrow} \tag{4.2.16}$$

$$\left[\hat{a}^\dagger_{-k\downarrow}, \sum_{n,\sigma} E_n b^\dagger_{n\sigma}b_{n\sigma}\right] = \sum_{n,\sigma} E_n \left[\hat{a}^\dagger_{-k\downarrow}, b^\dagger_{n\sigma}b_{n\sigma}\right]_- = 0 \tag{4.2.17}$$

$$\left[\hat{a}^\dagger_{-k\downarrow}, \sum_{nm\sigma\sigma'} J_{nm}b^\dagger_{n\sigma}b^\dagger_{m\sigma'}b_{m\sigma'}b_{n\sigma}\right] = \sum_{nm\sigma\sigma'} J_{nm} \left[\hat{a}^\dagger_{-k\downarrow}, b^\dagger_{n\sigma}b^\dagger_{m\sigma'}b_{m\sigma'}b_{n\sigma}\right]_+ = 0 \tag{4.2.18}$$

$$\left[\hat{a}^\dagger_{-k\downarrow}, U\sum_{\ell} n_{\ell\uparrow}n_{\ell\downarrow}\right] = U\sum_{\ell} \left[\hat{a}^\dagger_{-k\downarrow}, b^\dagger_{\ell\uparrow}b_{\ell\uparrow}b^\dagger_{\ell\downarrow}b_{\ell\downarrow}\right]_+ = 0 \tag{4.2.19}$$

$$\left[\hat{a}^\dagger_{-k\downarrow}, U'\sum_{\ell\ell'\sigma\sigma'} n_{\ell\sigma}n_{\ell'\sigma'}\right] = U'\sum_{\ell\ell'\sigma\sigma'} \left[\hat{a}^\dagger_{-k\downarrow}, b^\dagger_{\ell\sigma}b_{\ell\sigma}b^\dagger_{\ell'\sigma'}b_{\ell'\sigma'}\right]_+ = 0 \tag{4.2.20}$$

$$\left[\hat{a}^\dagger_{-k\downarrow}, \sum_{\ell mp} \Omega^{\ell m}_p b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}\hat{a}_{p\downarrow}\hat{a}_{p\uparrow}\right] = \sum_{\ell mp} \Omega^{\ell m}_p \left[\hat{a}^\dagger_{-k\downarrow}, b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}\hat{a}_{p\downarrow}\hat{a}_{-p\uparrow}\right]_+$$

$$= \sum_{\ell mp} \Omega^{\ell m}_p\{[\hat{a}^\dagger_{-k\downarrow}, b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}]\hat{a}_{p\downarrow}\hat{a}_{-p\uparrow} + b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{p\downarrow}\hat{a}_{-p\uparrow}]\}$$

$$= \sum_{\ell mp} \Omega^{\ell m}_p\{0 + b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}[\hat{a}^\dagger_{-k\downarrow}, \hat{a}_{p\downarrow}\hat{a}_{-p\uparrow}]\}$$

$$= \sum_{\ell m} \Omega^{\ell m}_{-k} b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}\hat{a}_{k\uparrow} \tag{4.2.21}$$

$$\left[\hat{a}^\dagger_{-k\downarrow}, \sum_{\ell mp} \Omega^{\ell m}_{k'} b_{m\downarrow}b_{\ell\uparrow}\hat{a}^\dagger_{-p\uparrow}\hat{a}^\dagger_{p\downarrow}\right] = \sum_{\ell mp} \Omega^{\ell m}_p \left[\hat{a}^\dagger_{-k\downarrow}, b_{m\downarrow}b_{\ell\uparrow}\hat{a}^\dagger_{-p\uparrow}\hat{a}^\dagger_{p\downarrow}\right]_+ = 0 \tag{4.2.22}$$

Substituting eqs.(4.2.15 - 4.2.22) into eq.(4.2.14), for $[\hat{a}^\dagger_{-k\downarrow}\hat{H}]$, we obtain

$$\omega\langle\langle\hat{a}^\dagger_{-k\downarrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle_\omega = -\epsilon_{-k}\langle\langle\hat{a}^\dagger_{-k\downarrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle - V\sum_p\langle\langle\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{k\uparrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle$$
$$+\sum_{\ell,m}\Omega^{\ell m}_{-k}\langle\langle b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}\hat{a}_{k\uparrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle \qquad (4.2.23)$$

Decoupling eq.(4.2.23), we get

$$\langle\langle\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\hat{a}_{k\uparrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle = \langle\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\rangle\langle\langle\hat{a}_{k\uparrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle \qquad (4.2.24a)$$

$$\langle\langle b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}\hat{a}_{k\uparrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle = \langle b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}\rangle\langle\langle\hat{a}_{k\uparrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle \qquad (4.2.24b)$$

Substituting eqs.(4.2.24a) and (4.2.24b) into eq.(4.2.23), we obtain

$$\omega\langle\langle\hat{a}^\dagger_{-k\downarrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle_\omega = -\epsilon_{-k}\langle\langle\hat{a}^\dagger_{-k\downarrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle - V\sum_p\langle\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\rangle\langle\langle\hat{a}_{k\uparrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle$$
$$+\sum_{\ell,m}\Omega^{\ell m}_{-k}\langle b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}\rangle\langle\langle\hat{a}_{k\uparrow},\hat{a}^\dagger_{k'\uparrow}\rangle\rangle$$

For k=k',

$$(\omega+\epsilon_{-k})\langle\langle\hat{a}^\dagger_{-k\downarrow},\hat{a}^\dagger_{k\uparrow}\rangle\rangle = -(\Delta^*-\eta^*)\langle\langle\hat{a}_{k\uparrow},\hat{a}^\dagger_{k\uparrow}\rangle\rangle \qquad (4.2.25)$$

where

$$\Delta^* = V\sum_p\langle\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow}\rangle$$

and

$$\eta^* = \sum_{k\ell m}\Omega^{\ell m}_{-k}\langle b^\dagger_{\ell\uparrow}b^\dagger_{m\downarrow}\rangle$$

From eq.(4.2.13), we obtain

$$\langle\langle\hat{a}_{k\uparrow},\hat{a}^\dagger_{k\uparrow}\rangle\rangle = \frac{1}{\omega-\epsilon_k}\left[\frac{1}{2\pi}-(\Delta-\eta)\langle\langle\hat{a}^\dagger_{-k\downarrow},\hat{a}^\dagger_{k\uparrow}\rangle\rangle\right] \qquad (4.2.26)$$

Substituting eq.(4.2.26) into eq.(4.2.25) for $\langle\langle\hat{a}_{k\uparrow},\hat{a}^\dagger_{k\uparrow}\rangle\rangle$ and rearranging, we get

$$\langle\langle\hat{a}^\dagger_{-k\downarrow},\hat{a}^\dagger_{k\uparrow}\rangle\rangle = -\frac{1}{2\pi}\left[\frac{\Delta-\eta}{\omega^2-\epsilon_k^2-(\Delta-\eta)^2}\right] \qquad (4.2.27)$$

and

$$\langle\langle \hat{a}_{k\uparrow}, \hat{a}^{\dagger}_{k\uparrow}\rangle\rangle = \frac{1}{2\pi}\left[\frac{\omega + \epsilon_k}{\omega^2 - \epsilon_k^2 - (\Delta - \eta)^2}\right] \tag{4.2.28}$$

where

$$\epsilon_k = \epsilon_{-k}$$

$$\Delta = \Delta^*$$

$$\eta = \eta^*$$

From eq.(4.2.27), we have

$$\langle\langle \hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k\uparrow}\rangle\rangle = -\frac{1}{2\pi}\left[\frac{\Delta - \eta}{\omega^2 - \epsilon_k^2 - (\Delta - \eta)^2}\right]$$

Using $\omega \longrightarrow i\omega_n$ in the above expression, we obtain

$$\langle\langle \hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k\uparrow}\rangle\rangle = -\frac{1}{2\pi}\left[\frac{\Delta - \eta}{(i\omega)^2 - \epsilon_k^2 - (\Delta - \eta)^2}\right]$$

$$\Longrightarrow \langle\langle \hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k\uparrow}\rangle\rangle = \frac{1}{2\pi}\left[\frac{\Delta - \eta}{\omega_n^2 + \epsilon_k^2 + (\Delta - \eta)^2}\right] \tag{4.2.29a}$$

From Matsubara's frequency for fermions, we have

$$\omega_n = \frac{(2n+1)\pi}{\beta} \tag{4.2.29b}$$

Substituting eq.(4.2.29b) into eq.(4.2.29a) for ω_n, we get

$$\langle\langle \hat{a}^{\dagger}_{-k\downarrow}, \hat{a}^{\dagger}_{k\uparrow}\rangle\rangle = \left[\frac{\beta^2(\Delta - \eta)}{(2n+1)^2\pi^2 + \beta^2[\epsilon_k^2 + (\Delta - \eta)^2]}\right] \tag{4.2.29c}$$

The superconducting order parameter(Δ) is given by

$$\Delta = \frac{V}{\beta}\sum_k \langle\langle \hat{a}^{\dagger}_{-k\downarrow}\hat{a}^{\dagger}_{k\uparrow}\rangle\rangle \tag{4.2.29d}$$

Substituting eq.(4.2.29c) into eq.(4.2.29d) for $\langle\langle \hat{a}_{-k\downarrow}, \hat{a}_{k\uparrow}\rangle\rangle$, we obtain

$$\Delta = \sum_{k,n} \frac{\beta V(\Delta - \eta)}{(2n+1)^2\pi^2 + \beta^2[\epsilon_k^2 + (\Delta - \eta)^2]} \qquad (4.2.29e)$$

Let

$$\epsilon_k^2 + (\Delta - \eta)^2 = \varepsilon_k^2 \qquad (4.2.29f)$$

and

$$\sum_{-\infty}^{\infty} \frac{1}{(2n+1)^2\pi^2 + \gamma_1^2} = \frac{\tanh \gamma_1/2}{2\gamma_1} \qquad (4.2.29g)$$

where $\gamma_1 = \beta\varepsilon_k$

Substituting eqs.(4.2.29f) and (4.2.29g) into eq.(4.2.29e), we get

$$\Delta = \sum_{k} \frac{V(\Delta - \eta)\tanh(\frac{\beta}{2}(\epsilon_k^2 + (\Delta - \eta)^2)^{\frac{1}{2}})}{2(\epsilon_k^2 + (\Delta - \eta)^2)^{\frac{1}{2}}} \qquad (4.2.29h)$$

Converting the summation over k values into an integral with the cut-off energy from $\pm\hbar\omega_b$ measured from the Fermi level and introducing the density of state at the fermi level (N(0)), we obtain

$$\Delta = N(0)V \int_{-\hbar\omega_b}^{\hbar\omega_b} (\Delta - \eta) \frac{\tanh(\frac{\beta}{2}[\epsilon_k^2 + (\Delta - \eta)^2]^{\frac{1}{2}})}{2[\epsilon_k^2 + (\Delta - \eta)^2]^{\frac{1}{2}}} d\epsilon_k$$

Let $\lambda = N(0)V$

$$\frac{1}{\lambda} = \int_{0}^{\hbar\omega_b} (1 - \frac{\eta}{\Delta}) \frac{\tanh[\frac{\beta}{2}(\epsilon_k^2 + (\Delta - \eta)^2)^{\frac{1}{2}}]}{(\epsilon_k^2 + (\Delta - \eta)^2)^{\frac{1}{2}}} d\epsilon_k \qquad (4.2.29I)$$

Eq.(4.2.29I) is analyzed for different values of the magnetic order parameter(η).

Now, let us study eq.(4.2.29I) by considering different cases

Case I. When $T \longrightarrow 0$, $\beta \longrightarrow \infty$,

Which implies,

$$\tanh(\frac{\beta}{2}[\epsilon_k^2 + (\Delta - \eta)^2]^{\frac{1}{2}}) \longrightarrow 1$$

Therefore, eq.(4.2.29I) becomes,

$$\frac{1}{\lambda} = \int_0^{\hbar\omega} \frac{1-\frac{\eta}{\Delta}}{(\epsilon_k^2 + (\Delta-\eta)^2)^{\frac{1}{2}}} d\epsilon_k \tag{4.2.29J}$$

$$\Longrightarrow \frac{1}{\lambda} = (1-\frac{\eta}{\Delta})\sinh^{-1}(\frac{\hbar\omega_b}{\Delta-\eta})$$

$$= (1-\frac{\eta}{\Delta})\ln\{\frac{\hbar\omega_b}{\Delta-\eta} + ((\frac{\hbar\omega_b}{\Delta-\eta})^2+1)^{\frac{1}{2}}\}$$

$$\simeq (1-\frac{\eta}{\Delta})\ln\frac{2\hbar\omega_b}{\Delta-\eta}$$

$$= (\Delta-\eta)2\hbar\omega_b \exp(-\frac{1}{\lambda(1-\frac{\eta}{\Delta})}) \tag{4.2.30}$$

When the magnetic ordering (η) is absent eq.(4.2.30) reduces to

$$\Delta = 2\hbar\omega_b \exp(-\frac{1}{\lambda}) \tag{4.2.31a}$$

From the BCS theory we have,

$$\frac{2\Delta(0)}{\kappa_B T_c} = 3.5$$

Therefore, eq.(4.2.31a) becomes

$$\kappa_B T_c = 1.14\hbar\omega_b \exp(-\frac{1}{\lambda}) \tag{4.2.31b}$$

which is the well known BCS expression for the superconducting transition temperature(T_c).

Case II. As $T \longrightarrow T_c$, $\Delta \longrightarrow 0$

From eq.(4.2.29I), we have

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} (1-\frac{\eta}{\Delta})\frac{\tanh[\frac{\beta}{2}(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}]}{(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}} d\epsilon_k \tag{4.2.32a}$$

$$\Longrightarrow \frac{1}{\lambda}=\int_0^{\hbar\omega_b}\frac{\tanh[\frac{\beta}{2}(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}]}{(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}}d\epsilon_k-\int_0^{\hbar\omega_b}\frac{\eta}{\Delta}\frac{\tanh[\frac{\beta}{2}(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}]}{(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}}d\epsilon_k \tag{4.2.32b}$$

Solving eq.(4.2.32b) using L'Hospitals's rule for $\Delta \longrightarrow 0$ as $T \longrightarrow T_c$, we get

$$\frac{1}{\lambda}=\int_0^{\hbar\omega_b}\lim_{\Delta\longrightarrow 0}\frac{\tanh[\frac{\beta}{2}(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}]}{(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}}d\epsilon_k-\int_0^{\hbar\omega_b}\lim_{\Delta\longrightarrow 0}(\frac{d}{d\Delta}\{\frac{\eta\tanh[\frac{\beta}{2}(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}]}{\Delta(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}}\}d\epsilon_k)$$

$$=\int_0^{\hbar\omega_b}\lim_{\Delta\longrightarrow 0}\frac{\tanh[\frac{\beta}{2}(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}]}{(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}}d\epsilon_k-\int_0^{\hbar\omega_b}\lim_{\Delta\longrightarrow 0}\frac{d}{d\Delta}\{\frac{\eta\tanh[\frac{\beta}{2}(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}]}{\Delta(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}}d\epsilon_k\}$$

$$=\int_0^{\hbar\omega_b}\frac{\tanh[\frac{\beta}{2}(\epsilon_k^2+\eta^2)^{\frac{1}{2}}]}{(\epsilon_k^2+\eta^2)^{\frac{1}{2}}}-\int_0^{\hbar\omega_b}\lim_{\Delta\longrightarrow 0}(\frac{d}{d\Delta}\{\frac{\eta\tanh[\frac{\beta}{2}(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}]}{\Delta(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}}\}d\epsilon_k$$

$$=\int_0^{\hbar\omega_b}\frac{\tanh[\frac{\beta}{2}(\epsilon_k^2+\eta^2)^{\frac{1}{2}}]}{(\epsilon_k^2+\eta^2)^{\frac{1}{2}}}-\int_0^{\hbar\omega_b}\lim_{\Delta\longrightarrow 0}(\eta\frac{\sec h^2[\frac{\beta}{2}(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}]\frac{\beta}{2}\frac{(\Delta-\eta)}{(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}}}{(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}+\frac{\Delta(\Delta-\eta)}{(\epsilon_k^2+(\Delta-\eta)^2)^{\frac{1}{2}}}})$$

$$\frac{1}{\lambda}=\int_0^{\hbar\omega_b}\frac{\tanh[\frac{\beta}{2}(\epsilon_k^2+\eta^2)^{\frac{1}{2}}]}{(\epsilon_k^2+\eta^2)^{\frac{1}{2}}}+\int_0^{\hbar\omega_b}\frac{\beta\eta^2}{2}\frac{\sec h^2[\frac{\beta}{2}(\epsilon_k^2+\eta^2)^{\frac{1}{2}}]}{(\epsilon_k^2+\eta^2)} \tag{4.2.33}$$

Eq.(4.2.33) is analyzed numerically for different combinations of the magnetic order parameter(η).

4.2.1. Equation Of Motion For The Localized Electrons

Now let us consider the equations of motion for the localized electrons

$$\omega\langle\langle b_{\ell\uparrow}, b^\dagger_{\ell'\uparrow}\rangle\rangle=\frac{\delta_{\ell\ell'}}{2\pi}+\langle\langle\left[b_{\ell\uparrow}\ \hat{H}\right], \hat{b}^\dagger_{\ell'\uparrow}\rangle\rangle \tag{4.2.34}$$

$$\left[b_{\ell\uparrow}, \sum_{k,\sigma}\epsilon_k\hat{a}^\dagger_{k\sigma}\hat{a}_{k\sigma}\right]=\sum_{k,\sigma}\epsilon_k\left[b_{\ell\uparrow}, \hat{a}^\dagger_{k\sigma}\hat{a}_{k\sigma}\right]_-=0 \tag{4.2.35}$$

$$\left[b_{\ell\uparrow}, V\sum_{k,k'}\hat{a}^\dagger_{k\uparrow}\hat{a}^\dagger_{-k\downarrow}\hat{a}_{-k'\downarrow}\hat{a}_{k'\uparrow}\right]=V\sum_{k,k'}\left[b_{\ell\uparrow}, \hat{a}^\dagger_{k\uparrow}\hat{a}^\dagger_{-k\downarrow}\hat{a}_{-k'\downarrow}\hat{a}_{k'\uparrow}\right]_+=0 \tag{4.2.36}$$

$$\left[b_{\ell\uparrow}, \sum_{n,\sigma}E_n b^\dagger_{n\sigma}b_{n\sigma}\right]=\sum_{n,\sigma}E_n\left[b_{\ell\uparrow}, b^\dagger_{n\sigma}b_{n\sigma}\right]_-=\sum_{n,\sigma}E_n(\left[b_{\ell\uparrow}, b^\dagger_{n\sigma}\right]b_{n\sigma}-0)$$

$$= E_\ell b_{\ell\uparrow} \tag{4.2.37}$$

$$\left[b_{\ell\uparrow}, \sum_{nm\sigma\sigma'} J_{nm} b^\dagger_{n\sigma} b^\dagger_{m\sigma'} b_{m\sigma'} b_{n\sigma}\right] = \sum_{nm\sigma\sigma'} J_{nm} \left[b_{\ell\uparrow}, b^\dagger_{n\sigma} b^\dagger_{m\sigma'} b_{m\sigma'} b_{n\sigma}\right]_+$$

$$= \sum_{nm\sigma\sigma'} J_{nm} \{[b_{\ell\uparrow}, b^\dagger_{n\sigma} b^\dagger_{m\sigma'}] b_{m\sigma'} b_{n\sigma} + b^\dagger_{n\sigma} b^\dagger_{m\sigma'} [b_{\ell\uparrow}, b_{m\sigma'} b_{n\sigma}]\}$$

$$= \sum_{nm\sigma\sigma'} J_{nm} \{[b_{\ell\uparrow}, b^\dagger_{n\sigma} b^\dagger_{m\sigma'}] b_{m\sigma'} b_{n\sigma} + 0\}$$

$$= \sum_{m,\sigma'} J_{\ell m} b^\dagger_{m\sigma'} b_{m\sigma'} b_{\ell\uparrow} \tag{4.2.38}$$

$$\left[b_{\ell\uparrow}, U \sum_{\ell'} n_{\ell'\uparrow} n_{\ell'\downarrow}\right] = U \sum_{\ell'} \left[b_{\ell\uparrow}, b^\dagger_{\ell'\uparrow} b_{\ell'\uparrow} b^\dagger_{\ell'\downarrow} b_{\ell'\downarrow}\right]_+$$

$$= U \sum_{\ell'} \{[b_{\ell\uparrow}, b^\dagger_{\ell'\uparrow} b_{\ell'\uparrow}] b^\dagger_{\ell'\downarrow} b_{\ell'\downarrow} + b^\dagger_{\ell'\uparrow} b_{\ell'\uparrow} [b_{\ell\uparrow}, b^\dagger_{\ell'\downarrow} b_{\ell'\downarrow}]\}$$

$$= U \sum_{\ell'} \{[b_{\ell\uparrow}, b^\dagger_{\ell'\uparrow} b_{\ell'\uparrow}] b^\dagger_{\ell'\downarrow} b_{\ell'\downarrow} + 0\}$$

$$= U \sum_{\ell'} \{\left[b_{\ell\uparrow}, b^\dagger_{\ell'\uparrow}\right] b_{\ell'\uparrow} - 0\} b^\dagger_{\ell'\downarrow} b_{\ell'\downarrow}$$

$$= U \sum b_{\ell\uparrow} b^\dagger_{\ell\downarrow} b_{\ell\downarrow} \tag{4.2.39}$$

$$\left[b_{\ell\uparrow}, U' \sum_{\ell'\ell''\sigma\sigma'} n_{\ell''\sigma} n_{\ell'\sigma'}\right] = U' \sum_{\ell'\ell''\sigma\sigma'} \left[b_{\ell\uparrow}, b^\dagger_{\ell''\sigma} b_{\ell''\sigma} b^\dagger_{\ell'\sigma'} b_{\ell'\sigma'}\right]_+$$

$$= U' \sum_{\ell'\ell''\sigma\sigma'} \{[b_{\ell\uparrow}, b^\dagger_{\ell''\sigma} b_{\ell''\sigma}] b^\dagger_{\ell'\sigma'} b_{\ell'\sigma'} + b^\dagger_{\ell''\sigma} b_{\ell''\sigma} [b_{\ell\uparrow}, b^\dagger_{\ell'\sigma'} b_{\ell'\sigma'}]\}$$

$$= U' \sum_{\ell'\ell''\sigma\sigma'} \{[b_{\ell\uparrow}, b^\dagger_{\ell''\sigma} b_{\ell''\sigma}] b^\dagger_{\ell'\sigma'} b_{\ell'\sigma'} + 0\}$$

$$= U' \sum_{\ell'\ell''\sigma\sigma'} \{\left[b_{\ell\uparrow}, b^\dagger_{\ell''\sigma}\right] b_{\ell''\sigma} - 0\} b^\dagger_{\ell'\sigma'} b_{\ell'\sigma'}$$

$$= U' \sum_{\ell',\sigma'} b_{\ell\uparrow} b^\dagger_{\ell'\sigma'} b_{\ell'\sigma'} \tag{4.2.40}$$

$$\left[b_{\ell\uparrow}, \sum_{\ell' m k} \Omega^{\ell' m}_k b^\dagger_{\ell'\uparrow} b^\dagger_{m\downarrow} \hat{a}_{k\downarrow} \hat{a}_{-k\uparrow}\right] = \sum_{\ell' m k} \Omega^{\ell' m}_k \left[b_{\ell\uparrow}, b^\dagger_{\ell'\uparrow} b^\dagger_{m\downarrow} \hat{a}_{k\downarrow} \hat{a}_{-k\uparrow}\right]_+$$

$$= \sum_{\ell' m k} \Omega^{\ell' m}_k \{[b_{\ell\uparrow}, b^\dagger_{\ell'\uparrow} b^\dagger_{m\downarrow}] \hat{a}_{k\downarrow} \hat{a}_{-k\uparrow} + b^\dagger_{\ell'\uparrow} b^\dagger_{m\downarrow} [b_{\ell\uparrow}, \hat{a}_{k\downarrow} \hat{a}_{-k\uparrow}]\}$$

$$= \sum_{\ell' m k} \Omega^{\ell' m}_k \{[b_{\ell\uparrow}, b^\dagger_{\ell'\uparrow} b^\dagger_{m\downarrow}] \hat{a}_{k\downarrow} \hat{a}_{-k\uparrow} + 0\}$$

$$= \sum_{m,k} \Omega^{\ell m}_k b^\dagger_{m\downarrow} \hat{a}_{k\downarrow} \hat{a}_{-k\uparrow} \tag{4.2.41}$$

$$\left[b_{\ell\uparrow},\sum_{\ell' mk}\Omega_k^{\ell' m}b_{m\downarrow}b_{\ell'\uparrow}\hat{a}^{\dagger}_{-k\uparrow}\hat{a}^{\dagger}_{k\downarrow}\right]=\sum_{\ell' mk}\Omega_k^{\ell' m}(\left[b_{\ell\uparrow},b_{m\downarrow}b_{\ell'\uparrow}\hat{a}^{\dagger}_{-k\uparrow}\hat{a}_{k\downarrow}\right]_{+}=0 \qquad (4.2.42)$$

Substituting eqs.(4.2.35 - 4.2.42) into eq.(4.2.34) for $[b_{\ell\uparrow},\hat{H}]$, we get

$$\omega\langle\langle b_{\ell\uparrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle_{\omega}=\frac{\delta_{\ell\ell'}}{2\pi}+E_{\ell}\langle\langle b_{\ell\uparrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle+\sum_{m,\sigma'}J_{\ell m}\langle\langle b^{\dagger}_{m\sigma'}b_{m\sigma'}b_{\ell\uparrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle+U\sum\langle\langle b_{\ell\uparrow}b^{\dagger}_{\ell\downarrow}b_{\ell\downarrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle$$

$$+U'\sum_{\sigma'}\langle\langle b_{\ell\uparrow}b^{\dagger}_{\ell'\sigma'}b_{\ell'\sigma'},b^{\dagger}_{\ell'\uparrow}\rangle\rangle+\sum_{km}\Omega_k^{\ell m}\langle\langle b^{\dagger}_{m\downarrow}\hat{a}_{k\downarrow}\hat{a}_{-k\uparrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle \qquad (4.2.43)$$

Decoupling the higher order Green's function of eq.(4.2.43) as

$$\langle\langle b^{\dagger}_{m\sigma'}b_{m\sigma'}b_{\ell\uparrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle=\langle b_{m\sigma'}b_{\ell\uparrow}\rangle\langle\langle b^{\dagger}_{m\sigma'},b^{\dagger}_{\ell'\uparrow}\rangle\rangle \qquad (4.2.44a)$$

$$\langle\langle b_{\ell\uparrow}b^{\dagger}_{\ell\downarrow}b_{\ell\downarrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle=\langle b_{\ell\uparrow}b_{\ell\downarrow}\rangle\langle\langle b^{\dagger}_{\ell\downarrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle \qquad (4.2.44b)$$

$$\langle\langle b_{\ell\uparrow}b^{\dagger}_{\ell'\sigma'}b_{\ell'\sigma'},b^{\dagger}_{\ell'\uparrow}\rangle\rangle=\langle b_{\ell\uparrow}b_{\ell'\sigma'}\rangle\langle\langle b^{\dagger}_{\ell'\sigma'},b^{\dagger}_{\ell'\uparrow}\rangle\rangle \qquad (4.2.44c)$$

$$\langle\langle b^{\dagger}_{m\downarrow}\hat{a}_{k\downarrow}\hat{a}_{-k\uparrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle=\langle\hat{a}_{k\downarrow}\hat{a}_{-k\uparrow}\rangle\langle\langle b^{\dagger}_{m\downarrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle \qquad (4.2.44d)$$

where $\sigma=\uparrow$ and $\sigma'=\downarrow$

and substituting eqs.(4.2.44a - 4.2.44d) into eq.(4.2.43), we get

$$(\omega-E_{\ell})\langle\langle b_{\ell\uparrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle=\frac{\delta_{\ell\ell'}}{2\pi}+\phi\langle\langle b^{\dagger}_{m\sigma'},b^{\dagger}_{\ell'\uparrow}\rangle\rangle+\varphi\langle\langle b^{\dagger}_{\ell\downarrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle+\psi\langle\langle b^{\dagger}_{\ell'\sigma'},b^{\dagger}_{\ell'\uparrow}\rangle\rangle$$

$$+\Gamma\langle\langle b^{\dagger}_{m\downarrow},b^{\dagger}_{\ell'\uparrow}\rangle\rangle$$

For $m = \ell' = \ell$, we obtain

$$(\omega-E_{\ell})\langle\langle b_{\ell\uparrow},b^{\dagger}_{\ell\uparrow}\rangle\rangle=\frac{1}{2\pi}+(\phi+\varphi+\psi+\Gamma)\langle\langle b^{\dagger}_{\ell\downarrow},b^{\dagger}_{\ell\uparrow}\rangle\rangle \qquad (4.2.45)$$

where

$$\phi=\sum_{\ell m\sigma'}J_{\ell m}\langle b_{m\sigma'}b_{\ell\uparrow}\rangle$$

$$\varphi=U\sum_{\ell}\langle b_{\ell\uparrow}b_{\ell\downarrow}\rangle$$

$$\psi=U'\sum_{\ell\ell'\sigma'}\langle b_{\ell\uparrow}b_{\ell'\sigma'}\rangle$$

$$\Gamma = \sum_{\ell mk} \Omega_k^{\ell m} \langle \hat{a}_{k\downarrow} \hat{a}_{-k\uparrow} \rangle$$

Similarly, the equation of motion for the higher order Green's function $\langle\langle b_{\ell\downarrow}^\dagger, b_{\ell'\uparrow}^\dagger \rangle\rangle$ can be obtained by evaluating the relevant commutators as shown below,

$$\omega \langle\langle b_{\ell\downarrow}^\dagger, b_{\ell'\uparrow}^\dagger \rangle\rangle_\omega = \langle\langle \left[b_{\ell\downarrow}^\dagger \ \hat{H} \right], b_{\ell'\uparrow}^\dagger \rangle\rangle \tag{4.2.46}$$

$$\left[b_{\ell\downarrow}^\dagger, \sum_{k,\sigma} \epsilon_k \hat{a}_{k\sigma}^\dagger \hat{a}_{k,\sigma} \right] = \sum_{k,\sigma} \epsilon_k \left[b_{\ell\downarrow}, \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} \right]_- = 0 \tag{4.2.47}$$

$$\left[b_{\ell\downarrow}^\dagger, V \sum_{k,k'} \hat{a}_{k\downarrow}^\dagger \hat{a}_{-k\downarrow}^\dagger \hat{a}_{-k'\downarrow} \hat{a}_{k'\uparrow} \right]_+$$

$$= V \sum_{k,k'} \{ [b_{\ell\downarrow}^\dagger, \hat{a}_{k\downarrow}^\dagger \hat{a}_{-k\downarrow}^\dagger] \hat{a}_{-k'\downarrow} \hat{a}_{k'\uparrow} + \hat{a}_{k\downarrow}^\dagger \hat{a}_{-k\downarrow}^\dagger [b_{\ell\downarrow}^\dagger, \hat{a}_{-k'\downarrow} \hat{a}_{k'\uparrow}] \}$$

$$= 0 \tag{4.2.48}$$

$$\left[b_{\ell\downarrow}^\dagger, \sum_{n,\sigma} E_n b_{n,\sigma}^\dagger b_{n\sigma} \right]_- = - \sum_{n,\sigma} E_n \left\{ 0 - \left[b_{\ell\downarrow}^\dagger, b_{n\sigma} \right] b_{n\sigma}^\dagger \right\}$$

$$= -E_\ell b_{\ell\downarrow}^\dagger \tag{4.2.49}$$

$$\left[b_{\ell\downarrow}^\dagger, \sum_{nm\sigma\sigma'} J_{nm} b_{n\sigma}^\dagger b_{m\sigma'}^\dagger b_{m\sigma'} b_{n\sigma} \right] = \sum_{nm\sigma\sigma'} J_{nm} [b_{\ell\downarrow}^\dagger, b_{n\sigma}^\dagger b_{m\sigma'}^\dagger b_{m\sigma'} b_{n\sigma}]_+$$

$$= \sum_{nm\sigma\sigma'} J_{nm} \{ [b_{\ell\downarrow}^\dagger, b_{n\sigma}^\dagger b_{m\sigma'}^\dagger] b_{n\sigma} b_{m\sigma'} + b_{n\sigma}^\dagger b_{m\sigma'}^\dagger [b_{\ell\downarrow}^\dagger, b_{m\sigma'} b_{n\sigma}] \}$$

$$= \sum_{nm\sigma\sigma'} J_{nm} \{ 0 + b_{n\sigma}^\dagger b_{m\sigma'}^\dagger [b_{\ell\downarrow}^\dagger, b_{m\sigma'} b_{n\sigma}] \}$$

$$= \sum_{nm\sigma\sigma'} J_{nm} b_{n\sigma}^\dagger b_{m\sigma'}^\dagger \{ \left[b_{\ell\downarrow}^\dagger, b_{m\sigma'} \right] b_{n\sigma} - 0 \}$$

$$= \sum_{n\sigma} J_{n\ell} b_{n\sigma}^\dagger b_{\ell\downarrow}^\dagger b_{n\sigma} \tag{4.2.50}$$

$$\left[b_{\ell\downarrow}^\dagger, U \sum n_{\ell\uparrow} n_{\ell\downarrow} \right] = U \sum_{\ell'} \left[b_{\ell\downarrow}^\dagger, b_{\ell'\uparrow}^\dagger b_{\ell'\uparrow} b_{\ell'\downarrow}^\dagger b_{\ell'\downarrow} \right]_+$$

$$= U \sum_{\ell'} \{ [b_{\ell\downarrow}^\dagger, b_{\ell'\uparrow}^\dagger b_{\ell'\uparrow}] b_{\ell'\downarrow}^\dagger b_{\ell'\downarrow} + b_{\ell'\uparrow}^\dagger b_{\ell'\uparrow} [b_{\ell\downarrow}^\dagger, b_{\ell'\downarrow}^\dagger b_{\ell'\downarrow}] \}$$

$$= U \sum_{\ell'} \{ 0 + b_{\ell'\uparrow}^\dagger b_{\ell'\uparrow} [b_{\ell\downarrow}^\dagger, b_{\ell'\downarrow}^\dagger b_{\ell'\downarrow}] \}$$

$$= -U \sum b_{\ell\uparrow}^\dagger b_{\ell\uparrow} b_{\ell\downarrow}^\dagger \tag{4.2.51}$$

$$\left[b^{\dagger}_{\ell\downarrow}, U' \sum_{\ell'\sigma\sigma'} n_{\ell'\sigma} n_{\ell''\sigma'}\right] = U' \sum_{\ell'\sigma\sigma'} [b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell'\sigma} b_{\ell'\sigma} b^{\dagger}_{\ell''\sigma'} b_{\ell''\sigma'}]_{+}$$

$$= U' \sum_{\ell'\sigma\sigma'} \{[b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell'\sigma} b_{\ell'\sigma}] b^{\dagger}_{\ell''\sigma'} b_{\ell''\sigma'} + b^{\dagger}_{\ell'\sigma} b_{\ell'\sigma} [b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell''\sigma'} b_{\ell''\sigma'}]\}$$

$$= U' \sum_{\ell'\sigma\sigma'} b^{\dagger}_{\ell'\sigma} b_{\ell'\sigma} b^{\dagger}_{\ell''\sigma'} \left[b^{\dagger}_{\ell\downarrow}, b_{\ell''\sigma'}\right]$$

$$= -U' \sum_{\sigma} b^{\dagger}_{\ell'\sigma} b_{\ell'\sigma} b^{\dagger}_{\ell\downarrow} \tag{4.2.52}$$

$$\left[b^{\dagger}_{\ell\downarrow}, \sum_{m,k} \Omega^{\ell m}_{k} b^{\dagger}_{\ell\uparrow} b^{\dagger}_{m\downarrow} \hat{a}_{k\downarrow} \hat{a}_{-k\uparrow}\right] = \sum_{m,k} \Omega^{\ell m}_{k} \left[b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell\uparrow} b^{\dagger}_{m\downarrow} \hat{a}_{k\downarrow} \hat{a}_{-k\uparrow}\right]_{+} = 0 \tag{4.2.53}$$

$$\left[b^{\dagger}_{\ell\downarrow}, \sum_{\ell' mk} \Omega^{\ell m}_{k} b_{m\downarrow} b_{\ell'\uparrow} \hat{a}^{\dagger}_{-k\uparrow} \hat{a}^{\dagger}_{k\downarrow}\right]_{+} = \sum_{\ell' mk} \Omega^{\ell' m}_{k} \{\left[b^{\dagger}_{\ell\downarrow}, b_{m\downarrow} b_{\ell'\uparrow}\right] \hat{a}^{\dagger}_{-k\uparrow} \hat{a}^{\dagger}_{k\downarrow}$$

$$+ b_{m\downarrow} b_{\ell'\uparrow} [b^{\dagger}_{\ell\downarrow}, \hat{a}^{\dagger}_{-k\uparrow} \hat{a}^{\dagger}_{k\downarrow}]\}$$

$$= \sum_{k,\ell'} \Omega^{\ell\ell'}_{k} b_{\ell'\uparrow} \hat{a}^{\dagger}_{-k\uparrow} \hat{a}^{\dagger}_{k\downarrow} \tag{4.2.54}$$

Substituting eqs.(4.2.47 - 4.2.54) into eq.(4.2.46) for $[b^{\dagger}_{\ell\downarrow} \hat{H}]$, we obtain

$$\omega \langle\langle b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle_{\omega} = \langle\langle -E_{\ell} b^{\dagger}_{\ell\downarrow} + \sum_{n\sigma\sigma'} J_{n\ell}\, b^{\dagger}_{n\sigma} b^{\dagger}_{\ell\downarrow} b_{n\sigma} - U \sum b^{\dagger}_{\ell\uparrow} b_{\ell\uparrow} b^{\dagger}_{\ell\downarrow}$$

$$-U' \sum_{\sigma} b^{\dagger}_{\ell'\sigma} b_{\ell'\sigma} b^{\dagger}_{\ell\downarrow} + \sum_{k} \Omega^{\ell'\ell}_{k} b_{\ell'\uparrow} \hat{a}^{\dagger}_{-k\uparrow} \hat{a}^{\dagger}_{k\downarrow}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle \tag{4.2.55}$$

Decoupling higher order Green's function of eq.(4.2.55) as

$$\langle\langle b^{\dagger}_{n\sigma} b^{\dagger}_{\ell\downarrow} b_{n\sigma}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle = \langle b^{\dagger}_{n\sigma} b^{\dagger}_{\ell\downarrow} \rangle \langle\langle b_{n\sigma}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle \tag{4.2.56a}$$

$$\langle\langle b^{\dagger}_{\ell\uparrow} b_{\ell\uparrow} b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle = \langle b^{\dagger}_{\ell\uparrow} b^{\dagger}_{\ell\downarrow} \rangle \langle\langle b_{\ell\uparrow}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle \tag{4.2.56b}$$

$$\langle\langle b^{\dagger}_{\ell'\sigma} b_{\ell'\sigma} b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle = \langle b^{\dagger}_{\ell'\sigma} b^{\dagger}_{\ell\downarrow} \rangle \langle\langle b_{\ell'\sigma}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle \tag{4.2.56c}$$

$$\langle\langle b_{\ell'\uparrow} \hat{a}^{\dagger}_{-k\uparrow} \hat{a}^{\dagger}_{k\downarrow}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle = \langle \hat{a}^{\dagger}_{-k\uparrow} \hat{a}^{\dagger}_{k\downarrow} \rangle \langle\langle b_{\ell'\uparrow}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle \tag{4.2.56d}$$

and substituting eqs.(4.2.56a - 4.2.56d) into eq.(4.2.55), we get

$$\omega \langle\langle b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle = -E_{\ell} \langle\langle b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle + \sum_{n,\sigma} J_{n\ell} \langle b^{\dagger}_{n\sigma} b^{\dagger}_{\ell\downarrow} \rangle \langle\langle b_{n\sigma}, b^{\dagger}_{\ell'\uparrow} \rangle\rangle$$

$$-U\sum\langle b^\dagger_{\ell\uparrow}b^\dagger_{\ell\downarrow}\rangle\langle\langle b_{\ell\uparrow},b^\dagger_{\ell'\uparrow}\rangle\rangle-U'\sum_\sigma\langle b^\dagger_{\ell'\sigma}b^\dagger_{\ell\downarrow}\rangle\langle\langle b_{\ell'\sigma},b^\dagger_{\ell'\uparrow}\rangle\rangle$$
$$+\sum_k\Omega_k^{\ell'\ell}\langle\hat{a}^\dagger_{-k\uparrow}\hat{a}^\dagger_{k\downarrow}\rangle\langle\langle b_{\ell'\uparrow},b^\dagger_{\ell'\uparrow}\rangle\rangle$$

Rearranging, we get

$$(\omega+E_\ell)\langle\langle b^\dagger_{\ell\downarrow},b^\dagger_{\ell'\uparrow}\rangle\rangle=(\phi^*-\varphi^*-\psi^*+\Gamma)\langle\langle b_{\ell'\uparrow},b^\dagger_{\ell'\uparrow}\rangle\rangle \tag{4.2.57}$$

where

$$\phi^*=\sum_{n\ell\sigma}J_{n\ell}\langle b^\dagger_{n\sigma}b^\dagger_{\ell\downarrow}\rangle$$
$$\varphi^*=U\sum_\ell\langle b^\dagger_{\ell\uparrow}b^\dagger_{\ell\downarrow}\rangle$$
$$\psi^*=U'\sum_{\ell',\sigma}\langle b^\dagger_{\ell'\sigma}b^\dagger_{\ell\downarrow}\rangle$$
$$\Gamma^*=\sum_{\ell\ell'k}\Omega_k^{\ell\ell'}\langle\hat{a}^\dagger_{-k\uparrow}\hat{a}^\dagger_{k\downarrow}\rangle$$

for

$$E_\ell=-E_\ell$$

$$\phi=\phi^*$$

$$\varphi=\varphi^*$$

$$\psi=\psi^*$$

$$\Gamma=\Gamma^*$$

and $\ell'=\ell$

we get

$$(\omega+E_\ell)\langle\langle b^\dagger_{\ell\downarrow},b^\dagger_{\ell\uparrow}\rangle\rangle=(\phi-\varphi-\psi+\Gamma)\langle\langle b_{\ell\uparrow},b^\dagger_{\ell\uparrow}\rangle\rangle \tag{4.2.58}$$

From eqs.(4.2.45) and (4.2.58), we get

$$\langle\langle b^\dagger_{\ell\downarrow},b^\dagger_{\ell\uparrow}\rangle\rangle=\frac{1}{2\pi}\left[\frac{\phi-\varphi-\psi+\Gamma}{\omega^2-E_\ell^2-(\phi-\varphi-\psi+\Gamma)(\phi+\varphi+\psi+\Gamma)}\right] \tag{4.2.59a}$$

and

$$\langle\langle b_{\ell\uparrow} b_{\ell\uparrow}^{\dagger}\rangle\rangle = \frac{1}{2\pi}\left[\frac{\omega + E_{\ell}}{\omega^2 - E_{\ell}^2 - (\phi - \varphi - \psi + \Gamma)(\phi + \varphi + \psi + \Gamma)}\right] \tag{4.2.59b}$$

Let

$$(\phi - \varphi - \psi + \Gamma)(\phi + \varphi + \psi + \Gamma) = \rho^2 \tag{4.2.60a}$$

and

$$\phi - \varphi - \psi + \Gamma = \chi_{\ell} \tag{4.2.60b}$$

Substituting eqs.(4.2.60a) and (4.2.60b) into eqs.(4.2.59a) and (4.2.59b) for ρ^2 and χ_{ℓ} , we obtain

$$\langle\langle b_{\ell\downarrow}^{\dagger}, b_{\ell\uparrow}^{\dagger}\rangle\rangle = \frac{1}{2\pi}\left[\frac{\chi_{\ell}}{\omega^2 - E_{\ell}^2 - \rho^2}\right] \tag{4.2.61a}$$

and

$$\langle\langle b_{\ell\uparrow}, b_{\ell\uparrow}^{\dagger}\rangle\rangle = \frac{1}{2\pi}[\frac{\omega + E_{\ell}}{\omega^2 - E_{\ell}^2 - \rho^2}] \tag{4.2.61b}$$

From eq.(4.2.61a), we have

$$\langle\langle b_{\ell\downarrow}^{\dagger}, b_{\ell\uparrow}^{\dagger}\rangle\rangle = \frac{1}{2\pi}\left[\frac{\chi_{\ell}}{\omega^2 - E_{\ell}^2 - \rho^2}\right] \tag{4.2.62a}$$

Let

$$\omega \longrightarrow i\omega_n \tag{4.2.62b}$$

Substituting eq.(4.2.62b) into eq.(4.2.62a) for ω, we obtain

$$\langle\langle b_{\ell\downarrow}^{\dagger}, b_{\ell\uparrow}^{\dagger}\rangle\rangle = -\frac{1}{2\pi}[\frac{\chi_{\ell}}{\omega_n^2 + E_{\ell}^2 + \rho^2}] \tag{4.2.62c}$$

Employing Matsubara's frequency for fermions which is given by

$$\omega_n = \frac{(2n+1)\pi}{\beta} \tag{4.2.62d}$$

we obtain

$$\langle\langle b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell\uparrow}\rangle\rangle = -\frac{\beta^2\chi_\ell}{(2n+1)^2\pi^2 + \beta^2 E_\ell^2 + \beta^2\rho^2} \tag{4.2.62e}$$

4.2.2. Correlation Between Conduction And Localized Electrons

Let

$$\eta = \sum_{\ell mk} \frac{\Omega^{\ell m}_{-k}}{\beta}\langle\langle b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell\uparrow}\rangle\rangle \tag{4.2.63a}$$

Substituting eq.(4.2.62e) into eq.(4.2.63a) for $\langle\langle b^{\dagger}_{\ell\downarrow}, b^{\dagger}_{\ell\uparrow}\rangle\rangle$, we get

$$\eta = -\sum_{\ell mk} \frac{\chi_\ell \beta \Omega^{\ell m}_{-k}}{(2n+1)^2\pi^2 + \beta^2(E_\ell^2 + \rho^2)} \tag{4.2.63b}$$

For

$$E_\ell^2 + \rho^2 = \zeta_\ell^2 \tag{4.2.63c}$$

and

$$\frac{\tanh \gamma_2/2}{2\gamma_2} = \sum_n \frac{1}{(2n+1)^2\pi^2 + \gamma_2^2} \tag{4.2.63d}$$

where $\gamma_2 = \beta\zeta_\ell$,

Substituting eqs.(4.2.63c) and (4.2.63d) into eq.(4.2.63b), we get

$$\eta = -\sum_\ell \chi_\ell \Omega^{\ell m}_{-k} \frac{\tanh(\frac{\beta}{2}(E_\ell^2 + \rho^2)^{\frac{1}{2}})}{2(E_\ell^2 + \rho^2)^{\frac{1}{2}}} \tag{4.2.64}$$

Converting summation into an integral with the cut-off energy from $\pm\hbar\omega_b'$ measured from the Fermi level and introducing the density of state N(ϵ_f), we obtain

$$\eta = -\chi_\ell \Omega^{\ell m}_{-k} N(\epsilon_f) \int_0^{\hbar\omega_b'} \frac{\tanh(\frac{\beta}{2}(E_\ell^2 + \rho^2)^{\frac{1}{2}})}{(E_\ell^2 + \rho^2)^{\frac{1}{2}}} dE_\ell \tag{4.2.65a}$$

Let $\Omega^{\ell m}_{-k} N(\epsilon_f) = \lambda_\ell$

Therefore, eq.(4.2.65a) becomes

$$\eta = -\chi_\ell \lambda_\ell \int_0^{\hbar\omega_b'} \frac{\tanh(\frac{\beta}{2}(E_\ell^2+\rho^2)^{\frac{1}{2}})}{(E_\ell^2+\rho^2)^{\frac{1}{2}}} dE_\ell \qquad (4.2.65b)$$

From which we obtain,

$$\eta = -\chi_\ell\lambda_\ell(\ln 1.14\frac{\hbar\omega_b'}{\kappa_B T_N} - \rho^2(\frac{1}{\kappa_B T_N})^2)\frac{11}{100}$$
$$= -\chi_\ell\lambda_\ell \ln 1.14\frac{\hbar\omega_b'}{\kappa_B T_N} + 0.11\chi_\ell\lambda_\ell\rho^2(\frac{1}{\kappa_B T_N})^2 \qquad (4.2.65c)$$

For $0.11\chi_\ell\lambda_\ell\rho^2 \longrightarrow 0$, eq.(4.2.65c) becomes

$$\eta = -\chi_\ell\lambda_\ell \ln 1.14\frac{\hbar\omega_b'}{\kappa_B T_N} \qquad (4.2.65d)$$

Finally, we obtain the following expression

$$\kappa_B T_N = 1.14\hbar\omega_b' \exp(\frac{\eta}{\chi_\ell\lambda_\ell})^1 \qquad (4.2.66)$$

[1] Derivation of eq.(4.2.66) is given in the Appendix

4.3 Results And Discussion

This part of our study deals with the investigation of the effect of magnetic ordering on the superconducting order parameter(Δ), on the transition temperature(T_c) and on the Ne'el or antiferromagnetic order temperature (T_N) in $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$. For this purpose, we consider a model Hamiltonian which contains interactions involving scattering of Cooper pairs by localized electrons of the gadolinium(Gd) ions which are the only magnetic species in $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$[122]. Using the model Hamiltonian and the double time temperature dependent Green's function formalism, we have obtained mathematical expressions for the superconducting order parameter (Δ), the transition temperature(T_c) and for the antiferromagnetic order temperature(T_N). Based on these expressions, we plot and discuss the phase diagrams for various combinations of these parameters.

4.3.1 *Phase Diagram Of Superconducting Order Parameter(Δ) Versus Temperature(T) For Various Values Of The Magnetic Order Parameter(η)*

The expression for the superconducting order parameter as a function of temperature and magnetic ordering has been obtained and is given in eq.(4.2.29I). It is analyzed numerically for various values of the magnetic order parameter(η). The phase diagram of the superconducting order parameter versus temperature for different values of the magnetic ordering is plotted. As can been seen from fig.4.1, the superconducting order parameter is suppressed when magnetic ordering is set in and this suppression becomes more significant as the value of the magnetic order parameter increases. This suppression could be attributed to the presence of magnetic ordering or magnetic impurity that scatters or flips the spins of the charge carriers by increasing the energy of the electrons involved in the Cooper pair and hence breaking up the pair.

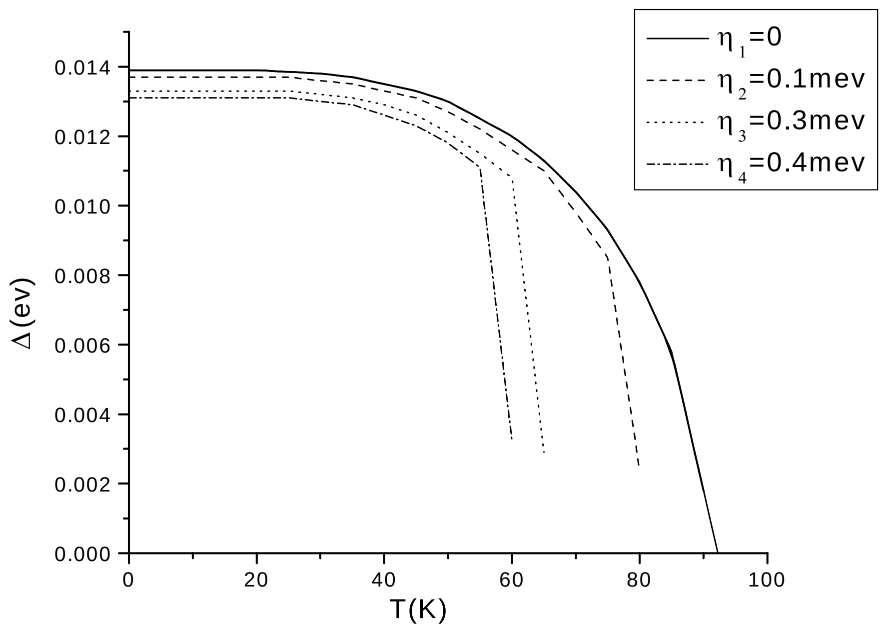

Fig. 4.1: Phase diagram of superconducting order parameter versus temperature for various values of the magnetic order parameter(eq.4.2.29I)

4.3.2 Phase Diagram Of Superconducting Transition Temperature (T_c) Versus Magnetic Order Parameter(η)

In this part of our study, we deal with the the effect of magnetic ordering on the transition temperature(T_c). Using eq.(4.2.33), the phase diagram of transition temperature versus magnetic ordering is plotted as shown in fig.(4.2). As can be seen from the figure, magnetic ordering suppresses the superconducting transition temperature(T_c). The suppression of T_c by magnetic ordering could be due to the coupling of the localized Gd 4f and the conduction Cu 3d and or oxygen 2p electrons that are sufficiently strong and results in the Cooper pair breaking effect which may be associated with the spin disorder scattering[110]. It is well known that, the way magnetic ordering influences superconductivity depends on the details of both the magnetic structure and the electron bands. That is, magnetic ordering does not destroy large pieces of the fermi surface since in the case of nesting, electronic properties are slightly modified and the opening of the magnetic gap does not cause drastic suppression on superconductivity[130].

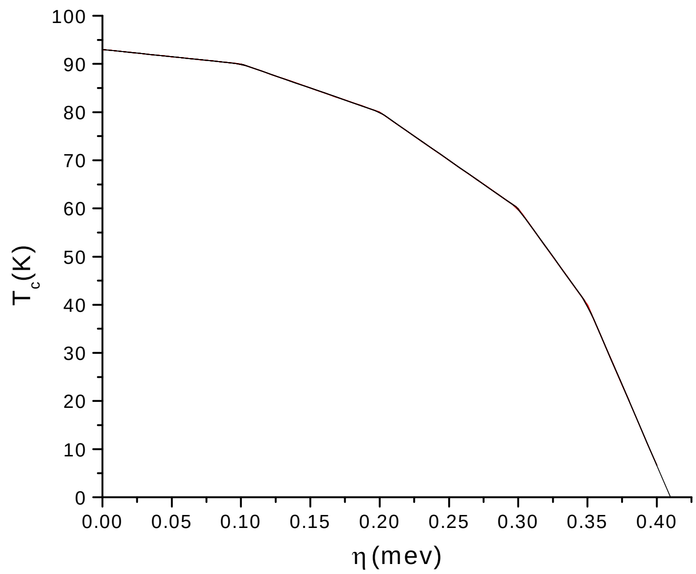

Fig. 4.2: Phase diagram of superconducting transition temperature versus magnetic order parameter(eq.4.2.33)

4.3.3 Phase Diagram Of Antiferromagnetic Order Temperature (T_N) Versus Magnetic Order Parameter(η)

The origin of magnetic ordering which results in the suppression of superconductivity is due to the quantum mechanical interaction between the spins of the localized electrons and atomic magnetic moments of the Gd ions. Below the transition temperature(T_c), the exchange interaction tries to align the Cooper pairs and hence exchange interaction causes stringent limits on the existence of superconductivity. Using eq.(4.2.66), the phase diagram of T_N versus η is plotted as given in fig.(4.3). Even though, magnetic ordering has the effect of suppressing both superconducting order parameter (Δ) and transition temperature(T_c), it has an effect of enhancing the Ne'el temperature(T_N) as shown in fig.4.3. This is probably because Gd is an s-state ion so that anisotropic crystal field effects arising from the Gd^{3+} ions may be absent. This implies that the antferromagnetic moment is in the basal plane for all values of η[17].

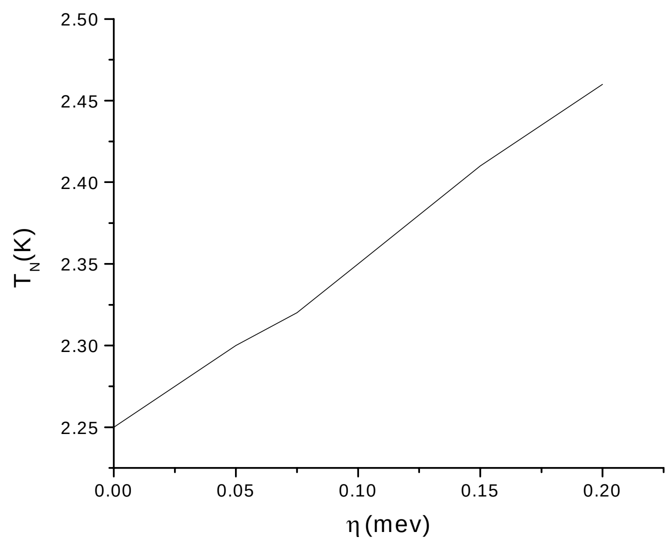

Fig. 4.3: Phase diagram of antiferromagnetic order temperature versus magnetic order parameter(eq.4.2.66)

Now, by merging figs. (4.2) and (4.3), we demonstrate the region where both superconductivity and antiferromagnetism coexist. This is illustrated in fig (4.4). Our investigation is in broad agreement with the experimental observations[110].

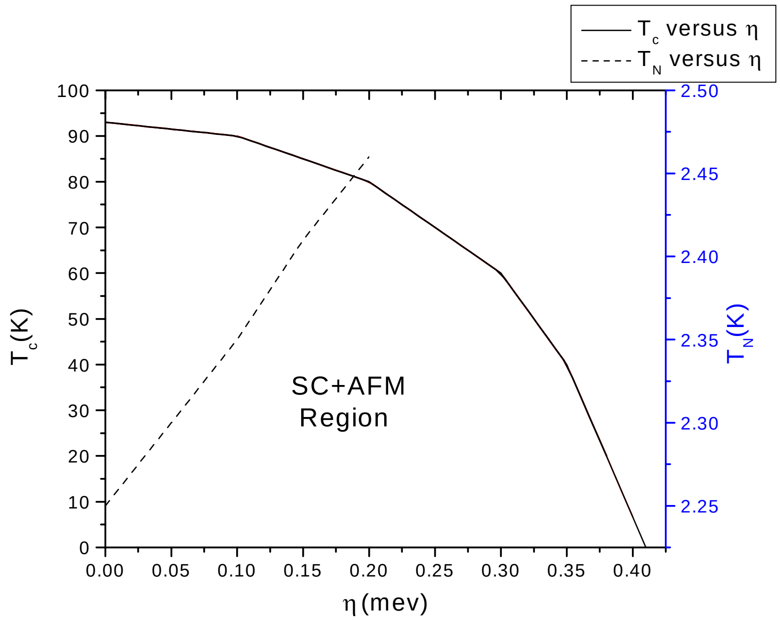

Fig. 4.4: Phase diagram of transition temperature and antiferromagnetic order temperature versus magnetic order parameter. The figure demonstrates the coexistence of superconductivity and antiferromagnetism(SC+AFM Region)

4.4 Coexistence Of Superconductivity And Ferromagnetism In UGe_2

4.4.1 *Introduction*

The problem of the interplay between ferromagnetic and superconducting long-range orders has recently attracted new interests due to the discovery of superconductivity in ferromagnetic materials such as UGe_2[4], $URhGe$[5], $ZrZn_2$[6] and in the ruthenocuprate $RuSr_2GdCu_2O_8$ compounds[64]. These two cooperative phenomena are mutually antagonistic because superconductivity is associated with the pairing of electron states related to time reversal, while in the magnetic states the time reversal symmetry is lost and hence there is a strong competition with superconductivity.

Experimental investigation by Matthias et al[60], demonstrated that, a very small concentration of magnetic impurities are enough to completely destroy superconductivity when ferromagnetic ordering is present[131].

Experiment by Saxena et al[4], demonstrated the existence of spin triplet superconducting states in the metallic compound UGe_2. This superconductivity is triggered by spontaneous magnetization of the ferromagnetic phase which exists at much higher temperatures and coexists with the superconducting phase in the whole domain of existence of the latter below T_c=1k[132]. Both the experiment and the theory favor parallel spin pairing, magnetically mediated superconductivity in these materials, but no microscopic material specific theory of superconductivity and magnetism coexistence exists at this time.

Correlation of superconductivity and magnetism has been one of the central issues in strongly correlated electron systems. In particular, one may find interesting materials showing the coexistence of superconductivity and ferromagnetic ordering in the uranium-based heavy fermion intermetallic compounds. These materials contain a periodic array of uranium ions[133].

In the recently discovered superconducting ferromagnetic compound UGe_2, the common belief is that the electrons responsible for the ferromagnetic ordering are the same which participate in the Cooper pair formation. That is, in UGe_2 both superconductivity and ferromagnetic ordering are carried by the U 5f-electrons. It is widely believed that, the attractive interaction between two electrons in a Cooper pair UGe_2 is mediated by magnetic excitations of the crystal lattice. Here, the spin of an electron travelling through the crystal lattice induces a magnetic dipole moment on the ions in the crystal lattice which in turn interacts with spin of a second electron passing in its vicinity. This leads to the formation of Cooper pairs consisting of two electrons with their spins aligned parallel to one another, that is, the triplet pairing.

4.4.2 Mathematical Formulation Of The Problem

To study the coexistence of superconductivity and ferromagnetism in UGe_2 ferromagnet, we consider the following generalized BCS Hamiltonian.

$$\hat{H} = \sum_{k,\sigma} \epsilon_k \hat{a}^{\dagger}_{k\sigma} \hat{a}_{k\sigma} + \frac{1}{2} \sum_{kk'} \sum_{\sigma 1 \sigma 2 \sigma 3 \sigma 4} V_{\sigma 1 \sigma 2 \sigma 3 \sigma 4}(kk')\ \hat{a}^{\dagger}_{\frac{q}{2}-k\sigma 1}\ \hat{a}^{\dagger}_{\frac{q}{2}+k\sigma 2}\ \hat{a}_{\frac{q}{2}+k'\sigma 3}\ \hat{a}_{\frac{q}{2}-k'\sigma 4}$$
$$- \sum_{\sigma,k} \sigma \mu \mathbf{H} \hat{a}^{\dagger}_{\sigma k} \hat{a}_{\sigma k} \qquad (4.4.1)$$

where ϵ_k denotes the band energy measured relative to the chemical potential(μ), $\mathbf{H}$ is the exchange field. $V_{\sigma 1 \sigma 2 \sigma 3 \sigma 4}(k, k')$ denotes the interaction potential matrix element

$$\langle -k\sigma_1;\ k\sigma_2 | V | -k'\sigma_4; k'\sigma_3 \rangle$$

with the following symmetry properties,

$$V_{\sigma 1 \sigma 2 \sigma 3 \sigma 4}(k, k') = -V_{\sigma 2 \sigma 1 \sigma 3 \sigma 4}(-k, k') = -V_{\sigma 1 \sigma 2 \sigma 4 \sigma 3}(k, -k') = V_{\sigma 4 \sigma 3 \sigma 2 \sigma 1}(k', k)\ .$$

and is attractive in a small energy range near the fermi surface for $-\epsilon_c \ \leq\ \epsilon(k)\ \leq \epsilon_c$, ϵ_c being the cut-off energy.

The superconductivity in this system is believed to be triplet regardless of the mechanism of pairing and can be achieved by a proper choice of spin indices $\sigma_1, \sigma_2, \sigma_3$ and σ_4. The pairing may be due to some unspecified mechanism possibly due to spin fluctuation as in He^3 and or electron-phonon coupling. This may allow interacting fermions to condense into fermion pairs with ℓ =1, 3, ..., states rather than into the specially symmetric, ℓ =0, s- state of the BCS theory.

We can obtain the mean field pair potential or gap function following Sigrist and Ueda[134] as follows.

$$\Delta_{\sigma\sigma'}(k) = -\sum_{k'\sigma 3 \sigma 4} V_{\sigma'\sigma\sigma 3 \sigma 4}(kk') \langle \hat{a}_{-k'\sigma 3} \hat{a}_{k'\sigma 4} \rangle \qquad (4.4.2)$$

and

$$\Delta^*_{\sigma\sigma'}(-k) = -\sum_{k'\sigma3\sigma4} V_{\sigma'\sigma\sigma3\sigma4}\hat{F}_{\sigma3\sigma4}(k',\beta) \tag{4.4.3}$$

The correlation $\langle \hat{a}_{k'\sigma3}\hat{a}_{-k'\sigma4}\rangle$ and $\langle \hat{a}^\dagger_{-k'\sigma1}\hat{a}^\dagger_{-k'\sigma2}\rangle$ can be calculated as,

$$\begin{aligned} F(k,\beta) &= \frac{1}{2E_{k\uparrow}}[d(k) + \frac{Q(k)\times d(k)}{|Q(k)|}]\tanh\frac{\beta}{2}E_\uparrow \\ &+\frac{1}{2E_{k\downarrow}}[d(k) - \frac{Q(k)\times d(k)}{|Q(k)|}]\tanh\frac{\beta}{2}E_\downarrow \end{aligned} \tag{4.4.4}$$

where, $E_{k\uparrow\downarrow} = [E_k^2 + |d(k)|^2 \pm Q(k)]^{\frac{1}{2}}$.

For the triplet state we have,

$$\Delta(k)\Delta^*(k) = |d(k)|^2\hat{I} + i\sigma Q(k)$$

with Q(k)= $(d(k)\times d^*(k))$

All the triplet states are non-unitary. For unitary states, $\Delta\Delta^*$ is proportional to unit matrix ($\hat{I}$). From the spectrum of E_k, we notice that there are two k-dependent gaps,

$E_k = [\epsilon_k'^2 + |d(k)|^2 \pm |d(k)\times d^*(k)|]^{\frac{1}{2}}$ in the energy spectrum.

For unitary pairing state ($Q(k) = 0$, for all k), hence $F(k,\beta)$ becomes,

$$F(k,\beta) = \frac{\Delta(k)}{E_k}\tanh\frac{\beta}{2}E_k \tag{4.4.5}$$

which produces the BCS or the s-wave superconductivity expression for T_c given by,

$$\kappa_B T_c = 1.14\hbar\omega_b' \exp(-\frac{1}{\lambda}) \tag{4.4.6}$$

where ω_b' is the boson excitation energy or spin fluctuation or any unspecified energy.

For a triplet state, we can obtain

$$\hat{F}(k, i\omega_n) = \frac{\{\omega_n^2 + [\epsilon_k^2 + |d(k)|^2]\}d(k) - iQ(k) \times d(k)}{(\omega_n^2 + E_{k+}^2)(\omega_n^2 + E_{k-}^2)} i\hat{\sigma}\sigma_y \tag{4.4.7}$$

For unitary pairing states, that is, for Q(k)=i(d(k)×$d^*(k)$)=0 and $E_{k\uparrow} = E_{k\downarrow}$, we have,

$$\hat{F}(k, \beta) = \Delta(k)[\frac{\tanh \frac{\beta}{2} E_{k\uparrow}}{2E_{k\uparrow}} + \frac{\tanh \frac{\beta}{2} E_{k\downarrow}}{2E_{k\downarrow}}] = \frac{\Delta(k)}{E_\uparrow} \tanh \frac{\beta}{2} E_{k\uparrow,\downarrow}$$

Using eqs. (4.4.3) and (4.4.4), we have

$$\Delta_{\sigma\sigma'} = \sum_{k'} V(kk')\{\frac{1}{2E_{k\uparrow}}[d(k) + \frac{Q(k) \times d(k)}{|Q(k)|}] \tanh \frac{\beta}{2} E_{k\uparrow}$$

$$+ \frac{1}{2E_{k\downarrow}}[d(k) - \frac{Q(k) \times d(k)}{|Q(k)|}] \tanh \frac{\beta}{2} E_{k\downarrow}\} \tag{4.4.8}$$

which can be re-cast into

$$1 = \sum N(\epsilon) V \frac{\tanh(\frac{\beta_c}{2}(E_k - \sigma\mu H))}{E_k - \sigma\mu\mathbf{H}}$$

where, $E_{k\uparrow,\downarrow} = E_k$

Here, we have taken energy dependent density of states.

Changing summation into integration, we obtain

$$1 = \int_0^{\hbar\omega_b'} V N(\epsilon) \frac{\tanh(\frac{\beta_c}{2}(E_k - \sigma\mu H))}{E_k - \sigma\mu\mathbf{H}} dE_k$$

For $z = \frac{\beta_c}{2}(E_k - \sigma\mu\mathbf{H})$, we get

$$\frac{1}{V[N(\epsilon_k)|_{\epsilon_f} \pm \frac{\partial N(\epsilon)}{\partial \epsilon}|_{\epsilon_f} \sigma\mu\mathbf{H}]} = \int_0^{\frac{2}{\beta}\hbar\omega_b'} \frac{\tanh z}{z} dz \tag{4.4.9}$$

Integrating eq.(4.4.9), we obtain

$$\kappa_B T_c = 1.14\hbar\omega_b' \exp\{-\frac{1}{V[N(\epsilon_k)|_{\epsilon_f} \pm \frac{\partial N(\epsilon)}{\partial \epsilon}|_{\epsilon_f} \sigma\mu\mathbf{H}]}\}$$

$$\Longrightarrow \kappa_B T_c = 1.14\hbar\omega_b' \exp\{-\frac{1}{V[N(\epsilon_k)|_{\epsilon_f} \pm \vartheta\sigma\mu\mathbf{H}]}\} \tag{4.4.10a}$$

where

$$\frac{\partial N(\epsilon)}{\partial \epsilon}|_{\epsilon_f} \;=\; \vartheta$$

Let

$$\lambda = VN(\epsilon)|_{\epsilon_f} \tag{4.4.10b}$$

and

$$\lambda' = V\sigma\mu\mathbf{H} \tag{4.4.10c}$$

Choosing, ϑ =1.

Substituting eqs.(4.4.10b) and (4.4.10c) into eq.(4.4.10a), we obtain

$$\kappa_B T_c = 1.14\hbar\omega_b' \exp(-\frac{1}{\lambda \pm \lambda'}) \tag{4.4.11}$$

From which we obtain,

$$\kappa_B T_{c\uparrow} = 1.14\hbar\omega_b' \exp(-\frac{1}{\lambda + \lambda'}) \tag{4.4.12a}$$

and

$$\kappa_B T_{c\downarrow} = 1.14\hbar\omega_b' \exp(-\frac{1}{\lambda - \lambda'}) \tag{4.4.12b}$$

4.4.3 *Variation Of Curie Temperature With Pressure And Coexistence Of Superconductivity And Ferromagnetism In UGe_2*

UGe_2 is known as a metallic ferromagnet with Curie temperature(T_m)=52K at ambient pressure[4,117]. That is, all the magnetic moments are aligned below 52K. However, as increasing pressure is applied to the system, the Curie temperature decreases rapidly and eventually vanishes at the critical pressure($P_c \geq$16kbar) due to the presence of a quantum critical point. The magnetization in UGe_2 is extremely anisotropic, with the easy a-axis in the orthorhombic crystal structure. The superconducting temperature(T_{sc}) shows a maximum value of 0.7K around a pressure of 12kbar. There is also another characteristic anomaly(cross-over) existing in UGe_2 at T^* in the ferromagnetic state residing below T_m. Application of pressure suppresses T^* to almost zero at a pressure of about 12kbar[120,126] where maximum superconducting transition temperature is also reached. By considering a free energy density appropriate to a triplet ferromagnet superconductor, the coexistence of superconductivity and ferromagnetism can be demonstrated[135].

The free energy functional(F)[136] can be written as,

F=$f_{no} + f_s + f_m + f_{sm}$

where f_{no} is the free energy functional of the normal state(that is, when the superconducting order parameter, $\psi' = 0$ and the ferromagnetic order parameter, M=0), f_s and f_m denote respectively the free energy functional for pure superconducting and ferromagnetic systems or states. f_{sm} is the free energy functional resulting from the coupling of ferromagnetic and superconducting parameters. For constant order parameters, that is, with no spacial variation and zero external magnetic field, these can be expressed as,

$$f_s = a|\psi'|^2 + \frac{b}{2}|\psi'|^4 \qquad (4.4.13a)$$

$$f_m = \alpha' M^2 + \frac{\beta'}{2} M^4 \qquad (4.4.13b)$$

$$f_{sm} = \eta' M^2 |\psi'|^2 - 4\pi SJM \qquad (4.4.13c)$$

where $S = i(\psi'^* \times \psi')$, b and β' are constants.

The last term in eq.(4.4.13c), denotes interaction of Cooper pair magnetization density with ferromagnetic magnetization density. This is important in a small pressure and temperature range where superconductivity exists.

It is assumed that,

$$a = a_o(\frac{T - T_{co}}{T_{co}})$$

$$\Longrightarrow a = a'_o(T - T_{co}) \qquad (4.4.14a)$$

and

$$\alpha = \alpha_o(\frac{T - T_{mo}}{T_{mo}})$$

$$\Longrightarrow \alpha = \alpha'_o(T - T_{mo}) \qquad (4.4.14b)$$

where

$$a'_o = \frac{a_o}{T_{co}}$$

and

$$\alpha'_o = \frac{\alpha_o}{T_{mo}}$$

As can be seen from eqs.(4.4.14a) and (4.4.14b), "a" and "α" change sign near the superconducting transition temperature(T_{co}) and ferromagnetic transition temperature(T_{mo}) respectively.

For arbitrary variation of F with respect to ψ' and M , we get

$$a + b|\psi'|^2 + \eta'|M|^2 = 0$$

and

$$\alpha + \beta' M^2 + \eta'|\psi'|^2 = 0$$

which can be solved to get expressions for the superconducting order parameter($|\psi'|^2$) and ferromagnetic order parameter (M^2)(linear in η') as coupling between superconducting and ferromagnetic order parameters is small and neglecting the coupling of Cooper pairs magnetization density with ferromagnetic magnetization density as

$$|\psi'|^2 = \frac{a_o}{b}(1 - \frac{T}{T_{co}}) - \frac{\alpha_o \eta'}{b\beta'}(1 - \frac{T}{T_{mo}}) \qquad (4.4.15a)$$

and

$$M^2 = \frac{\alpha_0}{\beta'}(1 - \frac{T}{T_{mo}}) - \frac{a_o \eta'}{b\beta'}(1 - \frac{T}{T_{co}}) \qquad (4.4.15b)$$

By letting $|\psi'|^2$ and $M^2 \longrightarrow 0$, at $T \longrightarrow T_c$ and $T \longrightarrow T_m$ respectively, we get

$$T_c = T_{co} - \frac{\eta'}{\beta'}\frac{\alpha_o}{a_o} T_{co}(1 - \frac{T_m}{T_{mo}}) \qquad (4.4.16a)$$

and

$$T_m = T_{mo} - \frac{a_o \eta' T_{mo}}{b\alpha_o}(1 - \frac{T_c}{T_{co}}) \qquad (4.4.16b)$$

where T_{co} and T_{mo} are respectively transition temperatures for superconducting and ferromagnetic materials in their pure states.

Several cases of interest can be examined depending on whether $T_{co} \longrightarrow T_{mo}$, $T_{co} < T_{mo}$ or $T_{co} > T_{mo}$.

For UGe_2 , T_{mo} is larger than T_{co} except in the neighborhood of the critical pressure(P_c) where superconductivity and ferromagnetism vanish.

From eqs.(4.4.13a) and (4.4.13b), the free energies for pure superconductivity and ferromagnetic states can be found to be $-\frac{a^2}{2b}$ and $-\frac{\alpha^2}{2\beta'}$ respectively.

Equating $-\frac{a^2}{2b}$ to $-\frac{\alpha^2}{2\beta'}$ at the ferromagnetic and superconducting interface, we get

$$\frac{a^2}{2b} = \frac{\alpha^2}{2\beta'}$$
$$\Longrightarrow \frac{a}{\sqrt{b}} = \frac{\alpha}{\sqrt{\beta'}}$$
$$\Longrightarrow a = \alpha\sqrt{\frac{b}{\beta'}}$$

leading to

$$T_{b'} = T_{co}(p) + \frac{\alpha_o'}{a_o'}\sqrt{\frac{b}{\beta'}}(T_{b'} - T_m(p)) \qquad (4.4.17)$$

where $T_{b'}$ is the temperature at the interface.

For $T_{mo} > T_{co}$ as is the case with UGe_2, the superconductivity will be under the umbrella of ferromagnetism.

Since superconductivity and ferromagnetism are coexisting in the triplet superconducting state as demonstrated by experiments, the coupling begins to acquire non-zero value as the Cooper pairs condense in the triplet state and this couples with ferromagnetic magnetization density of U 5f-electrons. At the interface or boundary, it is easy to show[134] that,

$$T_c(M) = T_{co} + \frac{4\pi JM}{a} + \eta' M^2|\psi'|^2 \qquad (4.4.18)$$

Here, $T_c(M)$ is the superconducting transition temperature with magnetization(M) developing and T_{co} is the superconducting transition temperature in the paramagnetic (M=0) state.

$$T_c(M) \simeq T_{co} + \frac{4\pi J}{a}\sqrt{\frac{\alpha'_o}{b\beta'}}[T_m(p) - T]^{\frac{1}{2}} + \frac{\alpha'_o\eta'}{b\beta'}[T_m(p) - T]a'_o[T_c(p) - T] \quad (4.4.19)$$

Here,

$$\frac{4\pi J}{a}\sqrt{\frac{\alpha'_o}{\beta'}}$$

has been identified with the cross- over temperature(T^*).

So, within the simple Ginzburg -Landau free energy functional as appropriate to our system, the phenomena of superconductivity and ferromagnetism is established. Therefore, superconductivity will be under the umbrella of ferromagnetism which can also be seen in [135].

1. **Variation Of Curie Temperature(T_m) With Pressure**:

As the ferromagnetic Curie temperature(T_m) goes to zero at a critical pressure(P_c), we can write

$$T_m(p) = T_m(0) + \alpha' P \quad (4.4.20)$$

So, at P=P_c, we have

$$T_m(p_c) = T_m(0) + \alpha' P_c = 0$$

$$\Longrightarrow T_m(0) + \alpha' P_c = 0$$

From which we obtain,

$$\alpha' = -\frac{T_m(0)}{P_c} \quad (4.4.21)$$

Substituting eq.(4.4.21) into eq.(4.4.20) for α' , we obtain

$$T_m(p) = T_m(0)[1 - \frac{P}{P_c}] \quad (4.4.22)$$

For UGe_2, $T_m(0)$ = 52K and P_c=16kbar[4,117]

2. **The Cross-Over Temperature(T^*)**

In order to find T^* the origin of which is not yet known we can use the following expression,

$$T^*(P) = T^*(0) + \gamma_3 P \qquad (4.4.23a)$$

As $T^*(p_{sc}) \simeq 0$ [4,117]

$T^*(0) + \gamma_3 P_{sc} = 0$

From which we get,

$$\gamma_3 = -\frac{T^*(0)}{P_{sc}} \qquad (4.4.23b)$$

Leading to

$$T^*(p) = T^*(0)[1 - \frac{P}{P_{sc}}] \qquad (4.4.24)$$

$T^*(0)$=30K and P_{sc}=12kbar for UGe_2[117]

3. **The Superconducting Temperature(T_{sc})**

Superconducting transition temperature can also be expressed as follows[135] provided that $T_{co}(0)$ is non-zero.

$$T_{sc}(p) = T_{co}(0)[1 - \frac{P}{P_{sc}}] \qquad (4.4.25)$$

4.5 Results And Discussion

4.4.4.1. In general a spin triplet superconductor is characterized by three pairing amplitudes or components of the order parameter corresponding to three symmetric combinations of spin

$| \uparrow\uparrow\rangle,\ | \downarrow\downarrow\rangle,$ and $| \uparrow\downarrow\rangle + | \downarrow\uparrow\rangle$.

A large spin splitting of the Fermion surfaces accompanied by suppression of singlet pairing may also suppress the last two of these components.

In UGe_2 it appears[4] that, the system exhibits ferromagnetism and superconductivity in which the superconductor attains $| \uparrow\uparrow\rangle$ state coexisting with ferromagnetism, whereas, the other spin states like $| \downarrow\downarrow\rangle$ and $\frac{1}{\sqrt{2}}(| \uparrow\downarrow\rangle + | \downarrow\uparrow\rangle)$ seem to have been washed out. This is the so called Anderson-Brinkman- Morel(ABM) state. The system may be staying in the mixed -Balian and Werthamer(BW) or ABM state with the preponderance of $| \uparrow\uparrow\rangle$ state. In He^3 two A and B phases have been identified with such phases[137]. To our mind, the mixed state, that is, spin singlet and spin triplet coexisting together has yet to be properly understood[137].

For appropriate parameters of UGe_2 superconductor, the phase diagrams of $T_{c\uparrow}$ and $T_{c\downarrow}$ spin states as a function of exchange field(splitting) of UGe_2 are plotted using eqs.(4.4.12a) and (4.4.12b) as shown in fig.4.5. It is believed that the density of state depends on the energy and on the exchange field(**H**) as the field splits the energy bands(levels) into two-one part for "spin up" electrons and one for "spin down" electrons. Since $T_{c\uparrow}$ is larger than $T_{c\downarrow}$, it would appear that the up spin(↑) electrons condense first and the down spin(↓) electrons remain unpaired. On further lowering of the temperature down spin (↓) electrons pair and undergo condensation and superconduct. With the existence of magnetic field of moderate strength, the two critical temperatures- $T_{c\uparrow}$ and $T_{c\downarrow}$ are clearly manifested[137] as shown in fig.(4.5).

For 3D ferromagnets in the absence of spin orbit coupling and for sufficient large splitting between the majority and minority spin fermi surfaces, the possibility of pairing opposite momentum states with antiparallel spins is virtually absent as states with opposite spins are no longer degenerate. Triplet pairing is the only channel available for pairing[5] with preponderance of spin triplet $\mid\uparrow\uparrow\rangle$ superconducting state. Specific heat measurements and the jump of ΔC at T_c can shed light if only one spin type of electrons undergoes superconducting pairing. Such an equal spin pairing(ESP)was predicted by Fay and Appel[138] for $ZrZn_2$ superconductor which is now known to be showing coexistence of ferromagnetism and superconductivity[6].

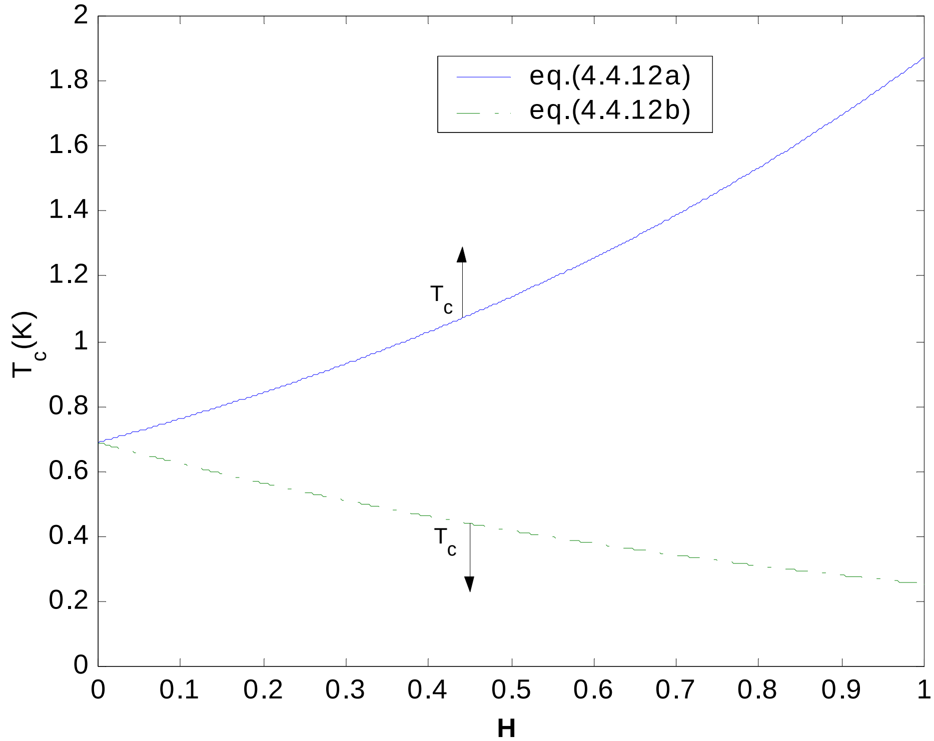

Fig. 4.5: Phase diagram of transition temperature(T_c) versus magnetic field($\mathbf{H}$) of UGe_2 (eqs.(4.4.12a) and (4.4.12b))

4.4.4.2. In this section, we discuss the variation of the Curie temperature(T_m) with pressure for UGe_2. Using eqs.(4.4.22), (4.4.24) and (4.4.25), we plot the phase diagram of the Curie temperature(T_m) versus pressure. As can be seen from the phase diagrams given in fig 4.6, the Curie temperature decreases monotonically with pressure. The decrease of T_m with pressure could be attributed to the quantum critical point, that is, since a small change in pressure destroys the magnetic ordering of atoms of solid materials such as UGe_2, the Curie temperature vanishes. This transition is driven solely by quantum fluctuations rather than thermal effects and are characterized by a critical pressure[59]. Furthermore, at ambient pressure the degree of delocalization of the f-electrons has been observed and pressure increases the extent of delocalization of the f-electrons as d_{u-u} is decreased. On the other hand, the increased uranium separation leads to a greater localization of the UGe_2 f-electrons. This may yield a possible mechanism for explaining the suppression of T_m with pressure[126]. In UGe_2 the same uranium 5f-electrons are involved in both ferromagnetism and superconductivity. This is manifested by the destruction of both ferromagnetism and superconductivity at the same pressure. As can be seen from fig.4.6, superconductivity is observed in the pressure range of 10-16kbar. Above the critical pressure, the system becomes paramagnetic with the loss of ferromagnetism. Hence, the coexistence of superconductivity and ferromagnetism is limited to a narrow region called the ferromagnetic fermi liquid(FMFL).

Our findings are in broad experimental agreement[4,117,120].

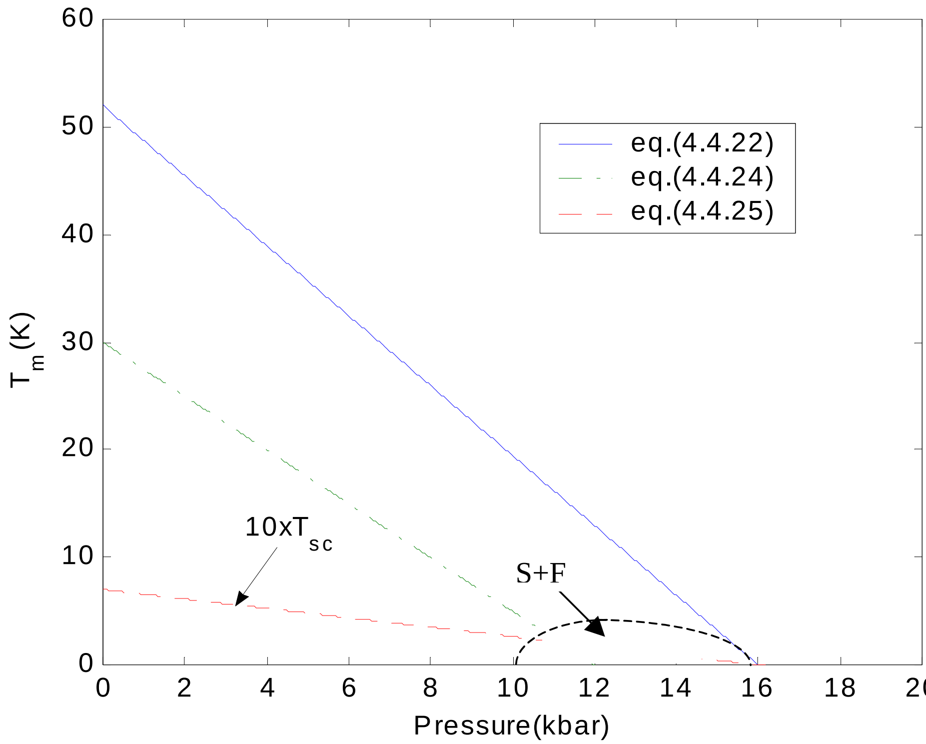

Fig. 4.6: Phase diagram of Curie temperature versus Pressure of UGe_2. The coexistence of superconductivity and ferromagnetism is observed in a narrow region(S+F)

5. SUMMARY AND CONCLUDING REMARKS

In the present research work, we have studied the possible coexistence of superconductivity and magnetism in $Ga_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$ and UGe_2. In the first two chapters, we have presented a brief introduction and a review of previous works which had been carried out by other researchers that are pertinent to our work. In Chapter 3, a brief review of the double time temperature dependent Green's function formalism, Zubarev[127] is presented. Chapter 4 is subdivided into two sections. In section 4.1, the coexistence of superconductivity and antiferromagnetism in $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$ is discussed by considering a model Hamiltonian. We have investigated the effect of magnetic order parameter(η) on superconductivity. For this purpose, the BCS formalism is extended to include interactions involving scattering of Cooper pairs by localized electrons of the Gd ions, intra and inter-atomic Coulomb interactions and exchange interaction. The expressions for the superconducting order parameter(Δ), transition temperature(T_c) and for antiferromagnetic ordering temperature(T_N) have been obtained. It has been found that superconductivity is suppressed when magnetic order parameter(η) sets in and the suppression becomes more significant when the antiferromagnetic correlations grow. Furthermore, T_c is observed to be suppressed when η is increased. This is verified by plotting the phase diagrams of superconducting order parameter(Δ) versus temperature(T) by varying the value of η and superconducting transition temperature(T_c) versus magnetic order parameter(η) as shown in figs. 4.1 and 4.2 respectively. On the other hand, in the orthorhombic state, magnetic ordering enhances the antiferromagnetic transition temperature(T_N) as indicated in the phase diagram of antiferromagnetic order temperature(T_N) versus magnetic order parameter(η)which is given in fig. 4.3. By merging figs. 4.2 and 4.3, we have found the region of coexistence of superconductivity and antiferromagnetism as shown in fig. 4.4.

In section 4.4, the coexistence of superconductivity and ferromagnetism in UGe_2 is presented. This is done by considering a generalized BCS Hamiltonian where the pairing could be due to any mechanism other than electron-phonon[134] and by employing the Green's function formalism. The effect of exchange field splits the energy bands into "spin up" and "spin down" electrons leading to condensation of up spin electrons at a higher T_c as shown in fig.4.5. On further lowering of the temperature, down spin electrons pair up and undergo condensation. Furthermore, the effect of pressure on the Curie temperature(T_m) of UGe_2 has been discussed. It has been shown that T_m decreases monotonically as pressure increases. We have also demonstrated the coexistence of superconductivity and ferromagnetism by plotting the phase diagram of T_m versus pressure as shown in fig.4.6. Close to the critical pressure(P_c) with $T_m(p)$ and $T_{sc}(p)$ approach zero which is indication of the fact that same uranium 5f-electrons are involved in producing superconductivity and ferromagnetism. In UGe_2 superconductor, the pairing is believed to be due to exchange of spin fluctuations. In this mechanism, the pairing results from the spin polarization of the medium. That is, an electron or a carrier with a particular orientation polarizes the spin medium and as a result another electron following is attracted by the spin polarization and hence form the spin triplet pairs which can then condense on lowering the temperature.

Finally, the coexistence of superconductivity and magnetism in $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$ and UGe_2 is demonstrated in the light of the proposed models for the two systems of superconductors - $Gd_{1+\eta}Ba_{2-\eta}Cu_3O_{7-\delta}$ and UGe_2 . The physical properties of URhGe at zero pressure closely resemble those of UGe_2 at high pressures(10-16kbar) where superconductivity is formed. In both of these superconductors, U f-electrons are implicitly involved in both highly correlated itinerant excitations and ferromagnetism.

Therefore, the superconductivity coexisting with ferromagnetism in URhGe can be understood in a similar way till more refined experiments are done on pure single crystals. The exact symmetry of the paired state and the dominant mechanism responsible for the pairing have also to be established beyond doubt before a better understanding of the two cooperative phenomena coexisting together is reached.

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APPENDIX

Derivation of eq.(4.2.66)

From eq.(4.2.66), we have

$$\eta = -\chi_\ell \lambda_\ell \int_0^{\hbar\omega_b'} \frac{\tanh(\frac{\beta}{2}(E_\ell^2+\rho^2)^{\frac{1}{2}})}{(E_\ell^2+\rho^2)^{\frac{1}{2}}} dE_\ell \qquad (A_1)$$

Integrating eq.(A_1), we get

$$\int_0^{\hbar\omega_b'} \frac{\tanh(\frac{\beta}{2}(\epsilon_k^2+\rho^2)^{\frac{1}{2}})}{(E_\ell^2+\rho^2)^{\frac{1}{2}}} dE_\ell = \int_0^{\hbar\omega_b'} dE_\ell \frac{2}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{\omega^2+E_\ell^2+\rho^2} \qquad (A_2)$$

Using the Laplace's transformation and the Matsubara frequency given by, $\omega_n = (2n+1)\frac{\pi}{\beta}$, eq.(A_2) becomes

$$= \int_0^{\hbar\omega_b'} dE_\ell \frac{2}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{\omega_n^2+E_\ell^2} - \int_0^{\hbar\omega_b'} \rho^2 \frac{2}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{(\omega_n^2+E_\ell^2)^2} + ...$$

$$= \int_0^{\hbar\omega_b'} \frac{\tanh\frac{\beta}{2}E_\ell}{E_\ell} dE_\ell - \int_0^{\hbar\omega_b'} \rho^2 dE_\ell \frac{2}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{(((2n+1)\frac{\pi}{\beta})^2+E_\ell^2)^2} + ... \qquad (A_3)$$

Let

$$\sum_{n=-\infty}^{\infty} \frac{1}{(((2n+1)\frac{\pi}{\beta})^2+E_\ell^2)^2} = 2\sum_{n=0}^{\infty} \frac{1}{(((2n+1)\frac{\pi}{\beta})^2+E_\ell^2)^2}$$

Let us now use the following relation

$$2\sum_{n=0}^{\infty} \frac{1}{(a^2+E_\ell^2)^2} = 2\sum_{n=0}^{\infty} \frac{1}{a^4(1+\frac{E_\ell^2}{a^2})^2} = 2\sum_{n=0}^{\infty} \frac{1}{a^4(1+x^2)^2} \qquad (A_4)$$

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

Hence, the integral of eq. (A_1) becomes

$$\int_0^{\hbar\omega_b'} \frac{\tanh(\frac{\beta}{2}(E_k^2+\rho^2)^{\frac{1}{2}})}{(E_\ell^2+\rho^2)^{\frac{1}{2}}} dE_\ell = \int_0^{\hbar\omega_b'} \frac{\tanh(\frac{\beta}{2}E_\ell)}{E_\ell} dE_\ell - \int_0^{\hbar\omega_b'} \rho^2 dE_\ell \frac{4}{\beta} \sum_{n=0}^{\infty} \frac{1}{a^4(1+x^2)^2} + ... \qquad (A_5)$$

$$= I_1 + I_2$$

where

$$I_1 = \int_0^{\hbar\omega_b'} \frac{\tanh(\frac{\beta}{2}E_\ell)}{E_\ell} dE_\ell$$

and

$$I_2 = \int_0^{\hbar\omega_b'} \rho^2 dE_\ell \frac{4}{\beta} \sum_{n=0}^{\infty} \frac{1}{a^4(1+x^2)^2} + ...$$

Now let us evaluate I_1

Let y=$\frac{\beta}{2}E_\ell$

$$= \int_0^{\frac{\beta}{2}\hbar\omega_b'} \frac{\tanh y}{y} dy$$

$$I_1 = \ln y \tanh y - \int_0^{\frac{\beta}{2}\hbar\omega_b'} \ln y \sec h^2 y dy \qquad (A_6)$$

For

$$\frac{\hbar\omega_b'}{2\kappa_B T_c} >> 1$$

we have

$$\tanh \frac{\hbar\omega_b'}{2\kappa_B T_c} \longrightarrow 1$$

Extending the upper limit of the integral in eq. (A_6) to infinity we get,

$$\int_0^{\infty} \ln y \sec h^2 y dy = \ln \frac{\pi}{4\gamma}$$

where $\gamma = \exp(0.577)$

Thus, eq. (A_6) becomes

$$I_1 = \ln \frac{\hbar\omega_b'}{2\kappa_B T_c} - \ln \frac{\pi}{4\gamma}$$

$$= \ln \frac{2\gamma}{\pi} \frac{\hbar\omega_b'}{\kappa_B T_c}$$

$$I_1 = \ln 1.14 \frac{\hbar\omega_b'}{\kappa_B T_c} \qquad (A_7)$$

Similarly, I_2 can be evaluated as follows

$$I_2 = \int_0^{\hbar\omega_b'} \rho^2 dE_\ell \frac{4}{\beta} \sum_{n=0}^{\infty} \frac{1}{a^4(1+x^2)^2} + ...$$

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

$$= \frac{4\beta^2}{\pi^3} \rho^2 \frac{7}{8} \zeta(3) \frac{\pi}{4}$$

$$I_2 = \rho^2 (\frac{1}{\kappa_B T_c})^2 \frac{11}{100} \qquad (A_8)$$

Eq. (A_8) is obtained by using the relations

$$\int_0^{\infty} \frac{dx}{(x^2+1)^2} = \frac{\pi}{4}$$

and

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

where r=3, $\zeta(r) = 1.202$ and is the Riemann Zeta-function

Now, substituting eqs.(A_1) and (A_8) into eq.(A_1), we obtain

$$\eta = -\chi_\ell \lambda_\ell \ln 1.14 \frac{\hbar\omega_b'}{\kappa_B T_N} + 0.11 \chi_\ell \lambda_\ell \rho^2 (\frac{1}{\kappa_B T_N})^2$$

$$\kappa_B T_N = 1.14 \hbar\omega_b' \exp(\frac{\eta - 0.11\chi_\ell \lambda_\ell \rho^2}{\chi_\ell \lambda_\ell}) \qquad (A_9)$$

Let $0.11\chi_\ell \lambda_\ell \rho^2 \longrightarrow 0$, then eq.$(A_9)$ becomes

$$\kappa_B T_N = 1.14 \hbar\omega_b' \exp(\frac{\eta}{\chi_\ell \lambda_\ell}) \qquad (A_{10})$$